



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:24 AM EDT

PDB ID : 4FQR / pdb_00004fqr
Title : Crystal structure of broadly neutralizing antibody C05 bound to H3 influenza hemagglutinin
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-06-25
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

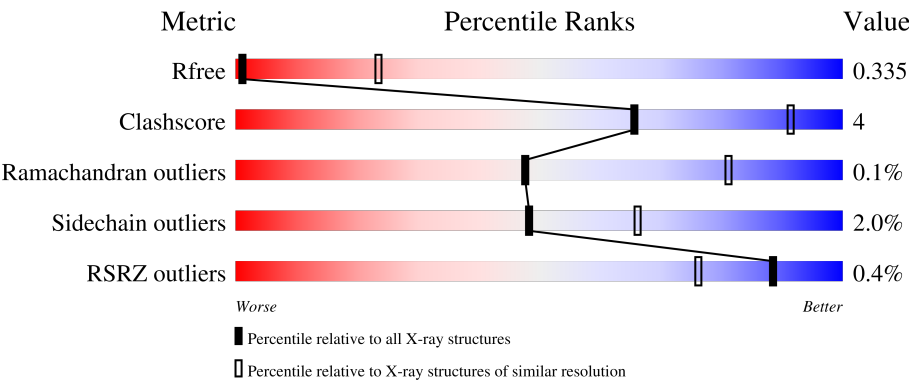
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



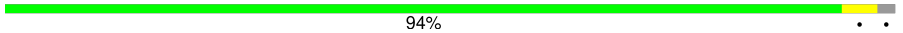
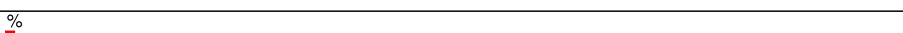
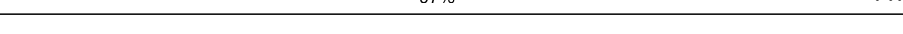
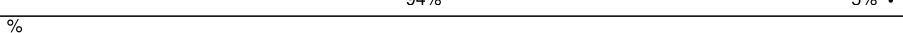
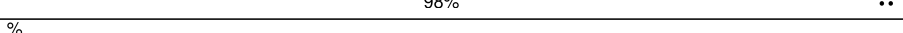
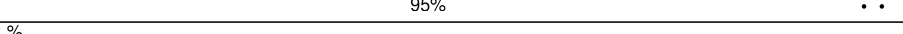
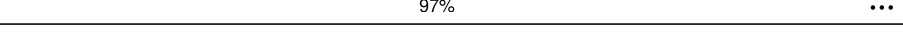
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	323	94% ...
1	C	323	93% 6% .
1	E	323	93% 5% .
1	G	323	% 93% 5% .
1	I	323	90% 7% ..

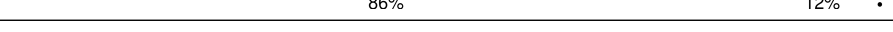
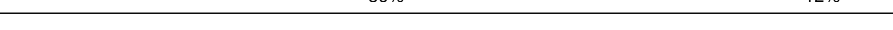
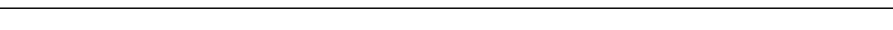
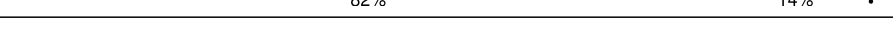
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Mol	Chain	Length	Quality of chain
1	K	323	 94% . .
1	M	323	 93% 5% . .
1	O	323	 91% 8% .
1	Q	323	 92% 6% .
1	S	323	 93% 5% .
1	U	323	 91% 7% .
1	W	323	 93% 6% .
2	B	174	 97% . .
2	D	174	 97% . .
2	F	174	 97% . . .
2	H	174	 95% . .
2	J	174	 97% . .
2	L	174	 98% . .
2	N	174	 97% . . .
2	P	174	 97% . . .
2	R	174	 94% 5% .
2	T	174	 98% . .
2	V	174	 95% . .
2	X	174	 97% . . .
3	a	241	 88% 10% . .
3	c	241	 89% 10% .
3	e	241	 88% 10% . .
3	g	241	 90% 7% . .
3	i	241	 84% 13% . .
3	k	241	 87% 12% .

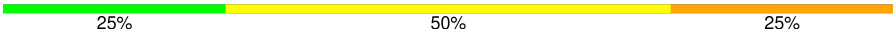
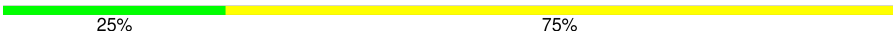
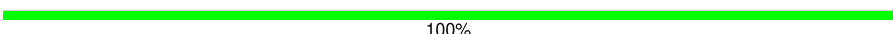
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Mol	Chain	Length	Quality of chain
3	m	241	 89% 9% .
3	o	241	 87% 12% ..
3	q	241	 86% 12% ..
3	s	241	 88% 10% ..
3	u	241	 87% 10% ..
3	w	241	 85% 13% ..
4	b	214	 88% 10% .
4	d	214	 85% 13% .
4	f	214	 87% 11% .
4	h	214	 86% 12% .
4	j	214	 86% 12% .
4	l	214	 86% 11% .
4	n	214	 86% 12% .
4	p	214	 82% 14% .
4	r	214	 87% 11% .
4	t	214	 86% 12% .
4	v	214	 86% 13% .
4	x	214	 86% 12% .
5	0	4	 50% 50%
5	2	4	 75% 25%
5	4	4	 75% 25%
5	6	4	 50% 50%
5	8	4	 50% 50%
5	AA	4	 50% 50%
5	CA	4	 75% 25%

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Mol	Chain	Length	Quality of chain
5	EA	4	
5	GA	4	
5	IA	4	
5	Y	4	
5	y	4	
6	1	2	
6	3	2	
6	5	2	
6	7	2	
6	9	2	
6	BA	2	
6	DA	2	
6	FA	2	
6	HA	2	
6	JA	2	
6	Z	2	
6	z	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 90792 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	C	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	E	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	G	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	I	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	K	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	M	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	O	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	Q	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	S	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	U	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	W	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7
G	7	ALA	-	expression tag	UNP Q91MA7
G	8	ASP	-	expression tag	UNP Q91MA7
G	9	PRO	-	expression tag	UNP Q91MA7
G	10	GLY	-	expression tag	UNP Q91MA7
I	7	ALA	-	expression tag	UNP Q91MA7
I	8	ASP	-	expression tag	UNP Q91MA7
I	9	PRO	-	expression tag	UNP Q91MA7
I	10	GLY	-	expression tag	UNP Q91MA7
K	7	ALA	-	expression tag	UNP Q91MA7
K	8	ASP	-	expression tag	UNP Q91MA7
K	9	PRO	-	expression tag	UNP Q91MA7
K	10	GLY	-	expression tag	UNP Q91MA7
M	7	ALA	-	expression tag	UNP Q91MA7
M	8	ASP	-	expression tag	UNP Q91MA7
M	9	PRO	-	expression tag	UNP Q91MA7
M	10	GLY	-	expression tag	UNP Q91MA7
O	7	ALA	-	expression tag	UNP Q91MA7
O	8	ASP	-	expression tag	UNP Q91MA7
O	9	PRO	-	expression tag	UNP Q91MA7
O	10	GLY	-	expression tag	UNP Q91MA7
Q	7	ALA	-	expression tag	UNP Q91MA7
Q	8	ASP	-	expression tag	UNP Q91MA7
Q	9	PRO	-	expression tag	UNP Q91MA7
Q	10	GLY	-	expression tag	UNP Q91MA7
S	7	ALA	-	expression tag	UNP Q91MA7
S	8	ASP	-	expression tag	UNP Q91MA7
S	9	PRO	-	expression tag	UNP Q91MA7
S	10	GLY	-	expression tag	UNP Q91MA7
U	7	ALA	-	expression tag	UNP Q91MA7
U	8	ASP	-	expression tag	UNP Q91MA7
U	9	PRO	-	expression tag	UNP Q91MA7
U	10	GLY	-	expression tag	UNP Q91MA7
W	7	ALA	-	expression tag	UNP Q91MA7
W	8	ASP	-	expression tag	UNP Q91MA7
W	9	PRO	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
W	10	GLY	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	D	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	F	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	H	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	J	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	L	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	N	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	P	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	R	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	T	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	V	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	X	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
D	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
F	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
H	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
J	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
L	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
N	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
P	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
R	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
T	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
V	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
X	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is a protein called Broadly neutralizing antibody C05, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	c	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	e	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	g	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	i	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	k	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	m	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	o	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	q	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	s	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	u	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	w	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			

- Molecule 4 is a protein called Broadly neutralizing antibody C05, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	b	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	d	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	f	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	h	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	l	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	n	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	p	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	r	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	t	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	v	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	x	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	y	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	0	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	2	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	4	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	6	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	8	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	AA	4	Total	C	N	O	0	0	0
			50	28	2	20			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	CA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	EA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	GA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	IA	4	Total	C	N	O	0	0	0
			50	28	2	20			

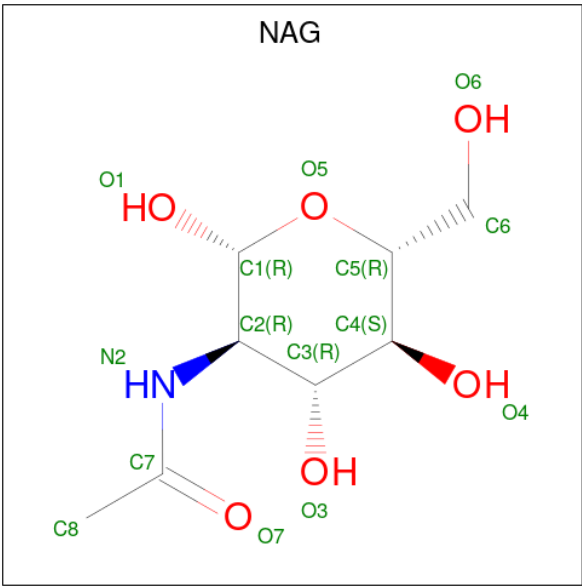
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	1	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	3	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	5	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	7	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	9	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	BA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	DA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	FA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	HA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	JA	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			14	8	1	5		
7	M	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		
7	O	1	Total	C	N	O	0	0
			14	8	1	5		
7	O	1	Total	C	N	O	0	0
			14	8	1	5		
7	P	1	Total	C	N	O	0	0
			14	8	1	5		
7	Q	1	Total	C	N	O	0	0
			14	8	1	5		
7	Q	1	Total	C	N	O	0	0
			14	8	1	5		
7	R	1	Total	C	N	O	0	0
			14	8	1	5		
7	S	1	Total	C	N	O	0	0
			14	8	1	5		
7	S	1	Total	C	N	O	0	0
			14	8	1	5		
7	T	1	Total	C	N	O	0	0
			14	8	1	5		
7	U	1	Total	C	N	O	0	0
			14	8	1	5		
7	U	1	Total	C	N	O	0	0
			14	8	1	5		
7	V	1	Total	C	N	O	0	0
			14	8	1	5		
7	W	1	Total	C	N	O	0	0
			14	8	1	5		
7	X	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Hemagglutinin HA1 chain

Chain A:  94% . .



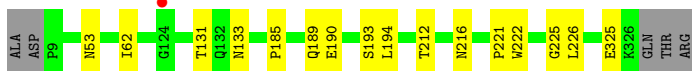
- Molecule 1: Hemagglutinin HA1 chain

Chain C:  93% 6% .

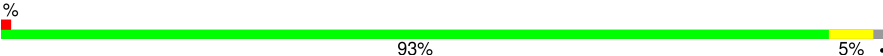


- Molecule 1: Hemagglutinin HA1 chain

Chain E:  93% 5% .



- Molecule 1: Hemagglutinin HA1 chain

Chain G:  93% 5% .

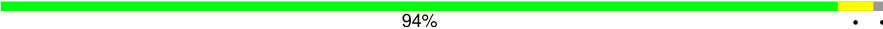


- Molecule 1: Hemagglutinin HA1 chain

Chain I:  90% 7% . .

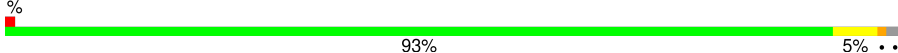


- Molecule 1: Hemagglutinin HA1 chain

Chain K:  94% . .



- Molecule 1: Hemagglutinin HA1 chain

Chain M:  93% 5% . .



- Molecule 1: Hemagglutinin HA1 chain

Chain O:  91% 8% .

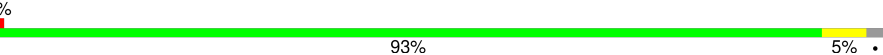


- Molecule 1: Hemagglutinin HA1 chain

Chain Q:  92% 6% .



- Molecule 1: Hemagglutinin HA1 chain

Chain S:  93% 5% .

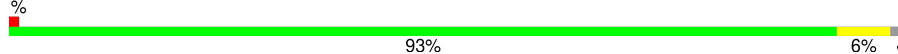


- Molecule 1: Hemagglutinin HA1 chain

Chain U:  91% 7% .



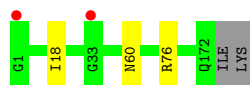
- Molecule 1: Hemagglutinin HA1 chain

Chain W:  93% 6% .

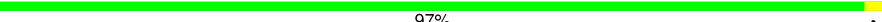


- Molecule 2: Hemagglutinin HA2 chain

Chain B:  97% ..



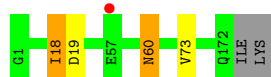
- Molecule 2: Hemagglutinin HA2 chain

Chain D:  97% ..



- Molecule 2: Hemagglutinin HA2 chain

Chain F:  97% ...



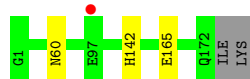
- Molecule 2: Hemagglutinin HA2 chain

Chain H:  95% ..

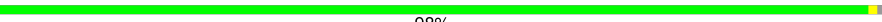


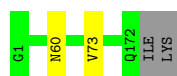
- Molecule 2: Hemagglutinin HA2 chain

Chain J:  97% ..



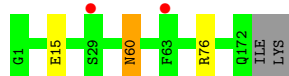
- Molecule 2: Hemagglutinin HA2 chain

Chain L:  98% ..

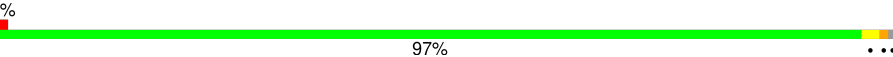


- Molecule 2: Hemagglutinin HA2 chain

Chain N:  97% ...



- Molecule 2: Hemagglutinin HA2 chain

Chain P:  97%

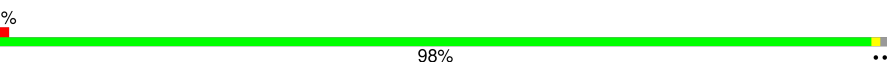


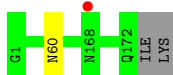
- Molecule 2: Hemagglutinin HA2 chain

Chain R:  94%

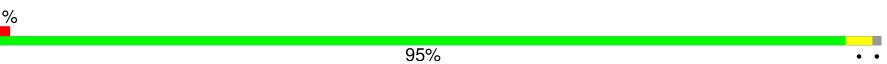


- Molecule 2: Hemagglutinin HA2 chain

Chain T:  98%

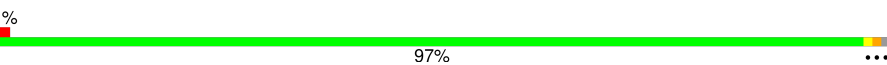


- Molecule 2: Hemagglutinin HA2 chain

Chain V:  95%



- Molecule 2: Hemagglutinin HA2 chain

Chain X:  97%



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain a:  88%



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain c:  89%



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain e:  88% 10% ..



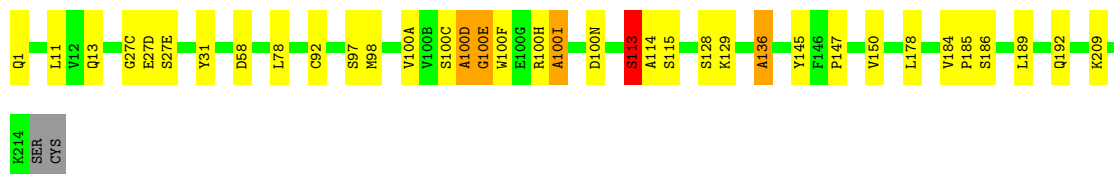
- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain g:  90% 7% ..



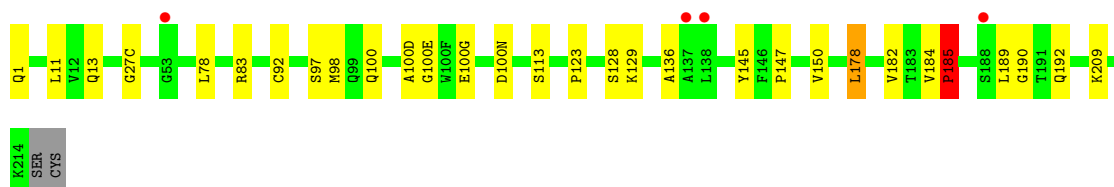
- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain i:  84% 13% ..



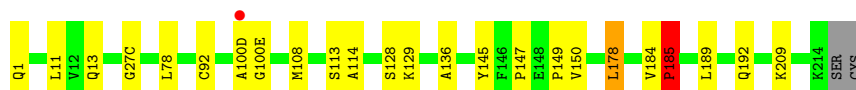
- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain k:  87% 12% .



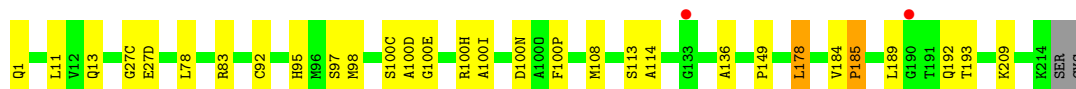
- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain m:  89% 9% .



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain o:  87% 12% ..



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain q:  86% 12% ..



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain s:  88% 10% ..



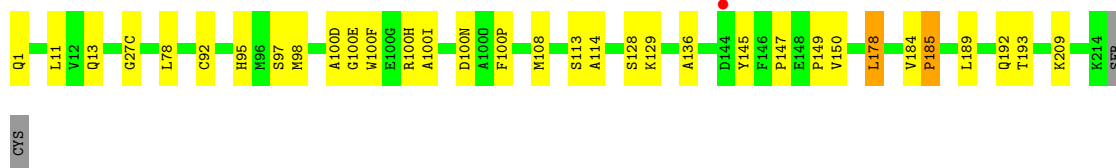
- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain u:  87% 10% ..



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain w:  85% 13% ..



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain b:  88% 10% .



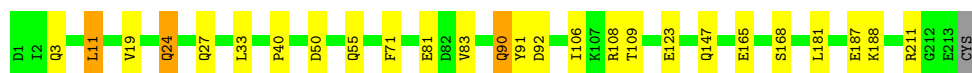
- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain d:  85% 13% .



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain f:  87% 11% .



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain h: 86% 12%



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain j: 86% 12%



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain l: 86% 11%



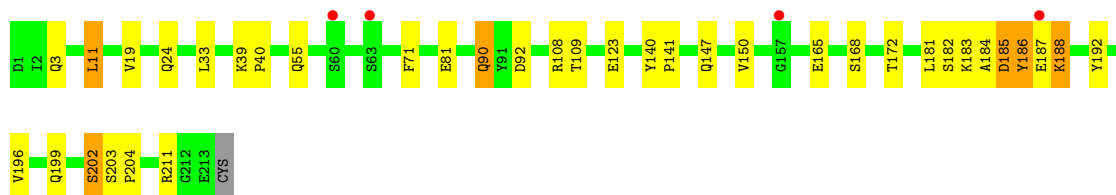
- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain n: 86% 12%



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain p: 2% 82% 14%



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain r: 87% 11%



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain t:  86% 12%



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain v:  86% 13%



- Molecule 4: Broadly neutralizing antibody C05, light chain

Chain x:  86% 12%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  75% 25%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:  75% 25%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  75% 25%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:  50% 50%

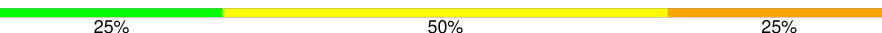


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:  75% 25%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:  25% 50% 25%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:  75% 25%

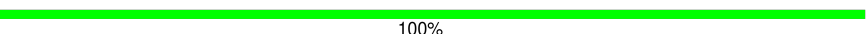


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:  75% 25%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:  50%  50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:  50%  50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:  50%  50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:  50%  50%

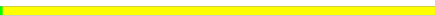


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:  50%  50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:  50%  50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA: 


MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	142.02Å 158.62Å 178.50Å 89.95° 85.44° 84.37°	Depositor
Resolution (Å)	49.07 – 4.10 49.07 – 4.10	Depositor EDS
% Data completeness (in resolution range)	73.9 (49.07-4.10) 58.9 (49.07-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.309 , 0.334 0.310 , 0.335	Depositor DCC
R_{free} test set	4527 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 596.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	90792	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1185e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, BMA, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/2612	0.80	2/3558 (0.1%)
1	C	0.50	0/2612	0.79	0/3558
1	E	0.49	0/2612	0.77	0/3558
1	G	0.50	0/2612	0.81	2/3558 (0.1%)
1	I	0.60	5/2612 (0.2%)	0.82	1/3558 (0.0%)
1	K	0.50	0/2612	0.78	1/3558 (0.0%)
1	M	0.57	4/2612 (0.2%)	0.87	4/3558 (0.1%)
1	O	0.52	1/2612 (0.0%)	0.79	1/3558 (0.0%)
1	Q	0.51	0/2612	0.79	3/3558 (0.1%)
1	S	0.49	0/2612	0.79	1/3558 (0.0%)
1	U	0.55	0/2612	0.82	2/3558 (0.1%)
1	W	0.52	1/2612 (0.0%)	0.78	0/3558
2	B	0.46	0/1470	0.78	1/1975 (0.1%)
2	D	0.46	0/1470	0.77	0/1975
2	F	0.52	1/1470 (0.1%)	0.82	1/1975 (0.1%)
2	H	0.47	0/1470	0.76	1/1975 (0.1%)
2	J	0.45	0/1470	0.77	0/1975
2	L	0.48	0/1470	0.78	0/1975
2	N	0.44	0/1470	0.77	1/1975 (0.1%)
2	P	0.47	0/1470	0.77	1/1975 (0.1%)
2	R	0.45	0/1470	0.77	1/1975 (0.1%)
2	T	0.45	0/1470	0.76	0/1975
2	V	0.46	0/1470	0.78	1/1975 (0.1%)
2	X	0.45	0/1470	0.76	1/1975 (0.1%)
3	a	0.63	1/1837 (0.1%)	0.90	5/2500 (0.2%)
3	c	0.54	0/1837	0.83	2/2500 (0.1%)
3	e	0.57	1/1837 (0.1%)	0.88	4/2500 (0.2%)
3	g	0.59	2/1837 (0.1%)	0.89	5/2500 (0.2%)
3	i	0.70	3/1837 (0.2%)	0.94	7/2500 (0.3%)
3	k	0.55	0/1837	0.85	3/2500 (0.1%)
3	m	0.54	0/1837	0.85	2/2500 (0.1%)
3	o	0.56	0/1837	0.85	5/2500 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	q	0.57	1/1837 (0.1%)	0.86	3/2500 (0.1%)
3	s	0.55	1/1837 (0.1%)	0.85	2/2500 (0.1%)
3	u	0.54	0/1837	0.87	7/2500 (0.3%)
3	w	0.55	0/1837	0.84	5/2500 (0.2%)
4	b	0.57	0/1682	0.80	2/2280 (0.1%)
4	d	0.65	0/1682	0.84	1/2280 (0.0%)
4	f	0.51	0/1682	0.78	0/2280
4	h	0.62	0/1682	0.83	0/2280
4	j	0.58	1/1682 (0.1%)	0.81	1/2280 (0.0%)
4	l	0.57	0/1682	0.79	1/2280 (0.0%)
4	n	0.61	1/1682 (0.1%)	0.79	0/2280
4	p	0.69	4/1682 (0.2%)	0.91	6/2280 (0.3%)
4	r	0.50	0/1682	0.77	0/2280
4	t	0.50	0/1682	0.77	1/2280 (0.0%)
4	v	0.62	0/1682	0.84	1/2280 (0.0%)
4	x	0.51	0/1682	0.79	2/2280 (0.1%)
All	All	0.54	27/91212 (0.0%)	0.82	90/123756 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
3	k	0	1
3	m	0	1
3	u	0	1
All	All	0	4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	100(D)	ALA	CA-CB	-10.14	1.37	1.53
4	p	183	LYS	N-CA	-7.36	1.37	1.46
3	i	100(D)	ALA	CA-CB	-7.13	1.42	1.53
1	M	20	VAL	CA-C	-7.11	1.46	1.52
3	g	116	THR	CB-CG2	-7.08	1.29	1.52
1	I	190	GLU	CA-CB	-7.00	1.42	1.53
4	p	182	SER	CA-C	-6.82	1.44	1.53
4	p	203	SER	N-CA	-6.76	1.39	1.45
3	e	100(D)	ALA	CA-CB	-6.75	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	190	GLU	CG-CD	-6.69	1.35	1.52
3	q	100(D)	ALA	CA-CB	-6.64	1.43	1.53
3	i	100(I)	ALA	CA-CB	-6.19	1.43	1.53
4	j	7	SER	CA-C	5.76	1.58	1.52
1	I	190	GLU	N-CA	-5.48	1.39	1.46
1	I	122	THR	CA-CB	-5.40	1.44	1.53
1	M	23	GLY	CA-C	5.37	1.57	1.51
2	F	18	ILE	CA-CB	-5.35	1.47	1.54
1	O	273	PRO	CA-C	-5.29	1.45	1.52
1	M	21	PRO	CA-C	5.28	1.59	1.52
3	s	100(D)	ALA	CA-CB	-5.28	1.45	1.53
1	M	20	VAL	N-CA	-5.26	1.42	1.46
4	n	110	VAL	CA-CB	5.24	1.59	1.54
3	i	136	ALA	CA-CB	-5.21	1.45	1.53
1	I	189	GLN	CA-C	-5.20	1.46	1.52
4	p	202	SER	CA-C	-5.12	1.45	1.52
3	g	189	LEU	CA-C	-5.09	1.46	1.52
1	W	190	GLU	CB-CG	-5.02	1.37	1.52

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	20	VAL	N-CA-C	-16.97	88.08	108.45
3	k	185	PRO	CA-C-O	-10.13	109.91	121.36
3	o	185	PRO	CA-C-O	-10.04	110.18	121.43
3	e	185	PRO	CA-C-O	-9.71	110.39	121.36
1	G	323	VAL	CA-C-N	-9.41	109.22	119.19
1	G	323	VAL	C-N-CA	-9.41	109.22	119.19
1	U	325	GLU	N-CA-C	9.35	124.62	109.85
4	p	182	SER	N-CA-C	9.29	122.80	110.53
1	S	226	LEU	N-CA-C	9.03	124.08	109.00
3	m	185	PRO	CA-C-O	-8.95	111.24	121.36
3	u	185	PRO	CA-C-O	-8.90	111.31	121.36
3	q	185	PRO	CA-C-O	-8.70	111.53	121.36
3	g	185	PRO	CA-C-O	-8.27	112.01	121.36
3	s	185	PRO	CA-C-O	-8.12	112.18	121.36
3	w	185	PRO	CA-C-O	-7.97	112.35	121.36
1	M	20	VAL	N-CA-CB	7.84	118.33	111.67
3	a	185	PRO	CA-C-O	-7.70	112.66	121.36
3	i	185	PRO	CA-C-O	-7.54	112.84	121.36
3	g	189	LEU	N-CA-C	7.49	119.23	111.14
4	p	186	TYR	N-CA-C	-7.25	102.56	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	i	100(E)	GLY	N-CA-C	7.03	124.72	114.10
1	M	226	LEU	N-CA-C	6.95	120.61	109.00
3	i	58	ASP	N-CA-C	6.90	119.65	109.24
3	a	192	GLN	N-CA-C	6.85	120.13	109.52
3	c	185	PRO	CA-C-O	-6.74	113.88	121.43
4	l	108	ARG	CA-C-O	-6.68	113.99	121.40
3	w	192	GLN	N-CA-C	6.63	119.80	109.52
3	u	192	GLN	N-CA-C	6.60	119.75	109.52
3	o	192	GLN	N-CA-C	6.58	119.72	109.52
1	I	190	GLU	CA-CB-CG	-6.56	100.99	114.10
4	p	185	ASP	N-CA-CB	6.54	119.84	110.16
4	p	183	LYS	N-CA-C	-6.38	104.33	111.28
3	q	192	GLN	N-CA-C	6.25	119.21	109.52
3	w	193	THR	N-CA-C	6.22	118.42	108.41
2	V	76	ARG	N-CA-C	6.21	118.56	111.11
2	P	76	ARG	N-CA-C	6.20	118.55	111.11
3	e	100(D)	ALA	N-CA-C	6.17	121.57	113.30
3	a	191	THR	N-CA-C	6.12	120.00	112.54
3	o	193	THR	N-CA-C	6.11	118.25	108.41
1	A	226	LEU	N-CA-C	6.10	119.10	109.15
1	O	46	SER	N-CA-C	6.09	118.95	109.52
3	c	192	GLN	N-CA-C	6.06	118.92	109.52
1	Q	226	LEU	N-CA-C	6.06	119.02	109.15
3	s	192	GLN	N-CA-C	6.02	118.85	109.52
3	e	66	ARG	N-CA-C	-6.00	105.86	113.43
1	K	226	LEU	N-CA-C	5.99	119.01	109.00
2	R	76	ARG	N-CA-C	5.89	118.18	111.11
2	H	76	ARG	N-CA-C	5.75	118.01	111.11
3	k	192	GLN	N-CA-C	5.74	118.41	109.52
2	B	76	ARG	N-CA-C	5.69	117.93	111.11
1	A	189	GLN	N-CA-C	5.66	117.12	111.07
3	i	113	SER	N-CA-C	5.65	119.43	112.54
3	i	192	GLN	N-CA-C	5.62	118.23	109.52
2	N	76	ARG	N-CA-C	5.62	117.85	111.11
3	m	192	GLN	N-CA-C	5.53	118.09	109.52
4	p	182	SER	CB-CA-C	-5.52	98.36	109.68
3	e	100(C)	SER	N-CA-C	-5.51	105.66	112.38
4	b	24	GLN	CB-CG-CD	-5.50	103.25	112.60
4	j	26	SER	N-CA-C	-5.49	106.54	113.18
3	a	58	ASP	N-CA-C	5.47	117.50	109.24
4	b	24	GLN	N-CA-C	5.45	117.78	108.90
1	Q	323	VAL	CA-C-N	-5.38	113.48	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	323	VAL	C-N-CA	-5.38	113.48	119.19
3	a	190	GLY	N-CA-C	-5.38	106.26	112.50
1	M	19	ALA	N-CA-C	-5.35	100.99	108.96
2	F	19	ASP	N-CA-C	5.33	119.34	112.41
4	v	126	LYS	N-CA-C	-5.30	105.45	112.34
3	g	201	LYS	CA-C-N	-5.29	113.46	119.28
3	g	201	LYS	C-N-CA	-5.29	113.46	119.28
4	d	126	LYS	N-CA-C	-5.28	105.48	112.34
3	k	190	GLY	N-CA-C	-5.26	106.42	112.83
4	x	108	ARG	N-CA-C	5.20	116.19	108.86
3	i	192	GLN	CA-C-N	5.20	129.33	122.42
3	i	192	GLN	C-N-CA	5.20	129.33	122.42
4	t	107	LYS	N-CA-C	-5.19	100.84	109.46
4	x	107	LYS	N-CA-C	-5.19	100.84	109.46
1	U	325	GLU	CB-CG-CD	-5.18	103.79	112.60
2	X	76	ARG	N-CA-C	5.13	117.26	111.11
4	p	184	ALA	CA-C-O	-5.11	115.64	121.00
3	u	192	GLN	CA-C-N	5.09	129.19	122.42
3	u	192	GLN	C-N-CA	5.09	129.19	122.42
3	u	189	LEU	CA-C-N	-5.08	114.35	119.98
3	u	189	LEU	C-N-CA	-5.08	114.35	119.98
3	q	193	THR	N-CA-C	5.06	116.56	108.41
3	u	193	THR	N-CA-C	5.05	116.55	108.41
3	w	192	GLN	CA-C-N	5.05	129.14	122.42
3	w	192	GLN	C-N-CA	5.05	129.14	122.42
3	g	184	VAL	N-CA-CB	-5.03	104.17	111.21
3	o	192	GLN	CA-C-N	5.02	129.10	122.42
3	o	192	GLN	C-N-CA	5.02	129.10	122.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	18	ILE	Mainchain
3	k	185	PRO	Mainchain
3	m	185	PRO	Mainchain
3	u	185	PRO	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2491	28	1
1	C	2553	0	2491	18	0
1	E	2553	0	2491	25	0
1	G	2553	0	2490	16	0
1	I	2553	0	2491	54	0
1	K	2553	0	2491	25	0
1	M	2553	0	2490	19	0
1	O	2553	0	2490	30	0
1	Q	2553	0	2490	31	0
1	S	2553	0	2490	24	0
1	U	2553	0	2490	26	3
1	W	2553	0	2491	24	0
2	B	1446	0	1370	1	0
2	D	1446	0	1370	2	0
2	F	1446	0	1370	2	0
2	H	1446	0	1370	3	0
2	J	1446	0	1370	1	0
2	L	1446	0	1370	1	0
2	N	1446	0	1370	2	0
2	P	1446	0	1370	2	0
2	R	1446	0	1370	4	0
2	T	1446	0	1370	0	0
2	V	1446	0	1370	2	0
2	X	1446	0	1370	2	0
3	a	1806	0	1749	32	0
3	c	1806	0	1749	18	0
3	e	1806	0	1749	33	0
3	g	1806	0	1749	21	0
3	i	1806	0	1749	52	0
3	k	1806	0	1749	34	0
3	m	1806	0	1749	25	0
3	o	1806	0	1749	32	0
3	q	1806	0	1749	35	0
3	s	1806	0	1749	28	0
3	u	1806	0	1749	28	0
3	w	1806	0	1749	29	0
4	b	1648	0	1614	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	1648	0	1614	21	1
4	f	1648	0	1614	15	0
4	h	1648	0	1614	15	4
4	j	1648	0	1614	15	1
4	l	1648	0	1614	18	1
4	n	1648	0	1614	16	1
4	p	1648	0	1614	22	1
4	r	1648	0	1614	14	0
4	t	1648	0	1614	18	0
4	v	1648	0	1614	19	1
4	x	1648	0	1614	13	0
5	0	50	0	43	0	0
5	2	50	0	43	0	0
5	4	50	0	43	0	0
5	6	50	0	43	0	0
5	8	50	0	43	0	0
5	AA	50	0	43	0	0
5	CA	50	0	43	0	0
5	EA	50	0	43	1	0
5	GA	50	0	43	0	0
5	IA	50	0	43	0	0
5	Y	50	0	43	0	0
5	y	50	0	43	0	0
6	1	28	0	25	0	0
6	3	28	0	25	0	0
6	5	28	0	25	0	0
6	7	28	0	25	0	0
6	9	28	0	25	0	0
6	BA	28	0	25	0	0
6	DA	28	0	25	0	0
6	FA	28	0	25	0	0
6	HA	28	0	25	0	0
6	JA	28	0	25	0	0
6	Z	28	0	25	0	0
6	z	28	0	25	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
7	E	14	0	13	0	0
7	F	14	0	13	0	0
7	G	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	14	0	13	0	0
7	I	14	0	13	0	0
7	J	14	0	13	0	0
7	K	14	0	13	0	0
7	L	14	0	13	0	0
7	M	28	0	26	0	0
7	N	14	0	13	0	0
7	O	28	0	26	0	0
7	P	14	0	13	0	0
7	Q	28	0	26	0	0
7	R	14	0	13	0	0
7	S	28	0	26	0	0
7	T	14	0	13	0	0
7	U	28	0	26	0	0
7	V	14	0	13	0	0
7	W	14	0	13	0	0
7	X	14	0	13	0	0
All	All	90792	0	87888	678	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (678) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD21	3:a:100(E):GLY:HA3	1.42	1.01
1:U:173:ASN:ND2	3:e:64:GLU:O	1.93	1.00
1:Q:226:LEU:HD21	3:q:100(E):GLY:HA3	1.42	0.99
1:Q:226:LEU:CD2	3:q:100(E):GLY:HA3	1.95	0.96
4:v:39:LYS:NZ	4:v:168:SER:OG	2.01	0.93
1:A:226:LEU:CD2	3:a:100(E):GLY:HA3	1.99	0.93
1:I:193:SER:HB3	3:i:98:MET:SD	2.11	0.90
1:I:98:TYR:OH	3:i:100(D):ALA:O	1.91	0.89
1:O:131:THR:OG1	3:o:100(H):ARG:NH2	2.06	0.89
1:W:131:THR:OG1	3:w:100(H):ARG:NH2	2.07	0.87
1:E:190:GLU:HG3	3:e:100(D):ALA:HB2	1.57	0.86
4:d:39:LYS:NZ	4:d:168:SER:OG	2.11	0.84
4:l:39:LYS:NZ	4:l:168:SER:OG	2.09	0.84
3:g:184:VAL:CG2	3:g:189:LEU:HD21	2.10	0.81
1:I:212:THR:HG21	1:K:216:ASN:CG	2.07	0.80
3:o:13:GLN:NE2	3:o:113:SER:O	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:GLU:CD	3:e:100(D):ALA:HB2	2.06	0.80
1:E:189:GLN:HG3	3:e:27(C):GLY:O	1.81	0.79
1:E:190:GLU:CG	3:e:100(D):ALA:HB2	2.12	0.79
1:A:226:LEU:HD21	3:a:100(E):GLY:CA	2.14	0.78
1:C:212:THR:HG21	1:E:216:ASN:ND2	1.99	0.78
3:i:13:GLN:NE2	3:i:113:SER:O	2.17	0.77
1:S:226:LEU:HD21	3:s:100(E):GLY:HA3	1.65	0.76
1:O:212:THR:HG21	1:Q:216:ASN:CG	2.11	0.75
1:E:131:THR:OG1	3:e:100(H):ARG:NH2	2.19	0.75
1:K:189:GLN:HG3	3:k:27(C):GLY:O	1.87	0.75
1:C:212:THR:HG21	1:E:216:ASN:CG	2.11	0.74
1:G:131:THR:OG1	3:g:100(H):ARG:NH2	2.20	0.74
1:K:226:LEU:HD21	3:k:100(E):GLY:CA	2.17	0.74
1:I:226:LEU:HD22	3:i:100(E):GLY:CA	2.18	0.73
1:M:226:LEU:HD21	3:m:100(E):GLY:N	2.04	0.72
4:n:39:LYS:NZ	4:n:168:SER:OG	2.20	0.72
1:I:189:GLN:HE21	3:i:27(E):SER:HA	1.52	0.72
1:O:189:GLN:HG3	3:o:27(C):GLY:O	1.90	0.72
1:U:212:THR:HG21	1:W:216:ASN:CG	2.15	0.72
1:A:216:ASN:CG	1:E:212:THR:HG21	2.14	0.71
1:S:226:LEU:HD21	3:s:100(E):GLY:CA	2.20	0.71
1:Q:190:GLU:CD	3:q:100(D):ALA:HB2	2.15	0.71
1:A:190:GLU:CD	3:a:100(D):ALA:HB2	2.15	0.71
1:K:226:LEU:HD21	3:k:100(E):GLY:HA3	1.73	0.71
1:M:189:GLN:NE2	3:m:27(C):GLY:O	2.24	0.70
1:S:226:LEU:HD21	3:s:100(E):GLY:N	2.06	0.70
3:g:116:THR:OG1	3:g:146:PHE:O	2.08	0.70
1:A:226:LEU:CD2	3:a:100(E):GLY:CA	2.69	0.69
4:p:185:ASP:HA	4:p:188:LYS:HB2	1.75	0.69
3:q:11:LEU:HB2	3:q:147:PRO:HG3	1.74	0.69
1:Q:226:LEU:HD21	3:q:100(E):GLY:CA	2.21	0.68
1:S:216:ASN:CG	1:W:212:THR:HG21	2.19	0.68
1:Q:137:ASN:ND2	3:q:100(G):GLU:OE1	2.26	0.68
4:h:50:ASP:OD1	4:h:91:TYR:OH	2.10	0.68
1:I:190:GLU:OE2	3:i:100(D):ALA:HB3	1.94	0.68
4:j:50:ASP:OD1	4:j:91:TYR:OH	2.10	0.68
3:o:97:SER:OG	3:o:100(N):ASP:OD2	2.06	0.68
1:I:212:THR:HG21	1:K:216:ASN:ND2	2.09	0.68
1:A:212:THR:HG21	1:C:216:ASN:CG	2.20	0.67
1:M:212:THR:HG21	1:O:216:ASN:CG	2.20	0.67
1:M:216:ASN:CG	1:Q:212:THR:HG21	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:LEU:CD2	3:i:100(E):GLY:HA3	2.25	0.67
1:M:226:LEU:HD21	3:m:100(E):GLY:HA3	1.78	0.66
1:Q:226:LEU:HD22	3:q:100(E):GLY:HA3	1.78	0.66
4:p:40:PRO:CB	4:p:165:GLU:HG3	2.25	0.66
1:O:212:THR:HG21	1:Q:216:ASN:ND2	2.10	0.66
1:M:226:LEU:HD21	3:m:100(E):GLY:CA	2.26	0.66
1:M:189:GLN:HG3	3:m:27(C):GLY:O	1.96	0.66
4:p:187:GLU:O	4:p:211:ARG:NH2	2.28	0.66
1:K:190:GLU:CD	3:k:100(D):ALA:HB2	2.21	0.65
4:p:40:PRO:HB2	4:p:165:GLU:HG3	1.77	0.65
1:I:214:ILE:HD11	1:K:216:ASN:HD21	1.60	0.65
1:W:189:GLN:HG3	3:w:27(C):GLY:O	1.97	0.65
4:l:12:SER:HB3	4:l:107:LYS:HE3	1.79	0.65
4:v:81:GLU:N	4:v:168:SER:O	2.29	0.65
1:G:212:THR:HG21	1:I:216:ASN:CG	2.22	0.65
1:K:189:GLN:NE2	3:k:27(C):GLY:O	2.30	0.65
1:S:212:THR:HG21	1:U:216:ASN:CG	2.21	0.65
4:x:50:ASP:OD1	4:x:91:TYR:OH	2.12	0.65
1:I:190:GLU:CD	3:i:100(D):ALA:HB3	2.22	0.64
1:I:226:LEU:CD2	3:i:100(E):GLY:CA	2.76	0.64
1:I:189:GLN:HG3	3:i:27(C):GLY:O	1.97	0.64
1:I:133:ASN:O	3:i:100(I):ALA:HB2	1.97	0.64
1:W:190:GLU:CG	3:w:100(D):ALA:HB2	2.28	0.64
1:S:137:ASN:ND2	3:s:100(G):GLU:OE1	2.30	0.64
1:A:216:ASN:ND2	1:E:212:THR:HG21	2.13	0.63
4:n:12:SER:HB3	4:n:107:LYS:HE3	1.80	0.63
1:S:190:GLU:CD	3:s:100(D):ALA:HB2	2.24	0.63
3:s:11:LEU:HB2	3:s:147:PRO:HG3	1.81	0.63
1:A:225:GLY:C	1:A:226:LEU:HD23	2.24	0.63
3:c:136:ALA:HB3	3:c:189:LEU:HD11	1.79	0.63
1:O:190:GLU:CG	3:o:100(D):ALA:HB2	2.29	0.63
1:U:212:THR:HG21	1:W:216:ASN:ND2	2.14	0.62
3:g:184:VAL:HG23	3:g:189:LEU:HD11	1.82	0.62
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.34	0.62
3:a:189:LEU:N	3:a:189:LEU:HD23	2.13	0.62
1:G:216:ASN:CG	1:K:212:THR:HG21	2.25	0.62
4:b:39:LYS:NZ	4:b:168:SER:OG	2.33	0.62
1:U:173:ASN:HD22	3:e:64:GLU:C	2.06	0.62
4:l:81:GLU:HA	4:l:168:SER:O	2.00	0.61
4:v:40:PRO:CB	4:v:165:GLU:HG3	2.30	0.61
1:Q:226:LEU:CD2	3:q:100(E):GLY:CA	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLN:HG3	3:c:27(C):GLY:O	1.99	0.61
1:M:216:ASN:ND2	1:Q:212:THR:HG21	2.15	0.61
1:Q:193:SER:HB3	3:q:98:MET:SD	2.41	0.61
1:S:216:ASN:ND2	1:W:212:THR:HG21	2.15	0.61
4:j:40:PRO:CB	4:j:165:GLU:HG3	2.30	0.61
4:h:40:PRO:CB	4:h:165:GLU:HG3	2.31	0.61
3:i:184:VAL:HG23	3:i:189:LEU:HD21	1.83	0.61
1:A:226:LEU:HD22	3:a:100(E):GLY:N	2.15	0.60
1:I:194:LEU:HD21	3:i:100(F):TRP:CE3	2.35	0.60
1:U:214:ILE:HD11	1:W:216:ASN:HD21	1.65	0.60
3:a:136:ALA:HB3	3:a:189:LEU:HD11	1.83	0.60
3:w:136:ALA:HB3	3:w:189:LEU:HD11	1.82	0.60
1:E:226:LEU:CD2	3:e:100(E):GLY:HA3	2.32	0.60
1:S:226:LEU:HD21	3:s:100(D):ALA:C	2.27	0.60
4:n:50:ASP:OD1	4:n:91:TYR:OH	2.17	0.60
1:W:190:GLU:HG3	3:w:100(D):ALA:HB2	1.83	0.60
1:M:212:THR:HG21	1:O:216:ASN:ND2	2.17	0.60
1:Q:190:GLU:CD	3:q:100(D):ALA:CB	2.75	0.59
1:U:131:THR:OG1	3:u:100(H):ARG:NH2	2.35	0.59
1:E:193:SER:HB3	3:e:98:MET:SD	2.42	0.59
1:O:214:ILE:HD11	1:Q:216:ASN:HD21	1.66	0.59
1:Q:222:TRP:CZ2	1:Q:225:GLY:HA2	2.37	0.59
4:j:81:GLU:HA	4:j:168:SER:O	2.03	0.59
1:E:133:ASN:O	3:e:100(I):ALA:HB2	2.02	0.59
1:I:190:GLU:OE1	3:i:100(D):ALA:CB	2.51	0.59
3:g:184:VAL:HG21	3:g:189:LEU:HD21	1.84	0.59
1:I:226:LEU:HD22	3:i:100(E):GLY:HA3	1.84	0.59
3:q:189:LEU:HD23	3:q:189:LEU:N	2.18	0.59
1:U:173:ASN:ND2	3:e:64:GLU:C	2.61	0.59
3:w:13:GLN:NE2	3:w:113:SER:O	2.35	0.59
1:I:190:GLU:HB2	3:i:100(A):VAL:HG11	1.85	0.59
1:M:136:SER:OG	3:m:100(E):GLY:O	2.18	0.59
1:G:216:ASN:ND2	1:K:212:THR:HG21	2.17	0.59
4:n:40:PRO:CB	4:n:165:GLU:HG3	2.33	0.59
3:i:136:ALA:HB3	3:i:189:LEU:HD11	1.85	0.58
1:A:212:THR:HG21	1:C:216:ASN:ND2	2.17	0.58
3:e:136:ALA:HB3	3:e:189:LEU:HD11	1.85	0.58
3:w:189:LEU:N	3:w:189:LEU:HD23	2.17	0.58
1:I:190:GLU:CB	3:i:100(A):VAL:HG11	2.34	0.58
1:I:222:TRP:CZ2	1:I:225:GLY:HA2	2.38	0.58
4:d:123:GLU:HA	4:d:126:LYS:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:189:LEU:N	3:m:189:LEU:HD23	2.17	0.58
3:k:189:LEU:N	3:k:189:LEU:HD23	2.18	0.58
1:I:193:SER:CB	3:i:98:MET:SD	2.89	0.58
1:O:193:SER:HB3	3:o:98:MET:SD	2.44	0.58
1:I:226:LEU:HD22	3:i:100(E):GLY:N	2.19	0.57
1:S:189:GLN:CG	3:s:27(C):GLY:O	2.52	0.57
4:f:81:GLU:HA	4:f:168:SER:O	2.04	0.57
1:I:228[B]:SER:OG	3:i:100(D):ALA:HA	2.05	0.57
1:Q:189:GLN:HG3	3:q:27(C):GLY:O	2.05	0.57
3:k:184:VAL:HG23	3:k:189:LEU:CD1	2.34	0.57
3:m:11:LEU:HB2	3:m:147:PRO:HG3	1.85	0.57
1:E:226:LEU:HD21	3:e:100(E):GLY:CA	2.35	0.57
1:S:212:THR:HG21	1:U:216:ASN:ND2	2.19	0.57
3:w:11:LEU:HB2	3:w:147:PRO:HG3	1.87	0.57
1:I:190:GLU:OE1	3:i:100(D):ALA:HB2	2.05	0.57
1:K:189:GLN:CG	3:k:27(C):GLY:O	2.53	0.57
4:d:81:GLU:HA	4:d:168:SER:O	2.04	0.57
3:c:189:LEU:N	3:c:189:LEU:HD23	2.20	0.56
1:I:189:GLN:NE2	3:i:31:TYR:CZ	2.73	0.56
1:S:189:GLN:HG3	3:s:27(C):GLY:O	2.04	0.56
3:s:97:SER:OG	3:s:100(N):ASP:OD2	2.17	0.56
1:I:190:GLU:CG	3:i:100(A):VAL:HG11	2.36	0.56
4:p:90:GLN:OE1	4:p:92:ASP:N	2.38	0.56
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.40	0.56
1:I:189:GLN:NE2	3:i:27(E):SER:HA	2.18	0.56
1:U:173:ASN:HB3	3:e:64:GLU:OE1	2.06	0.56
4:n:81:GLU:HA	4:n:168:SER:O	2.05	0.56
3:u:189:LEU:N	3:u:189:LEU:HD23	2.19	0.56
4:x:40:PRO:CB	4:x:165:GLU:HG3	2.35	0.56
1:O:190:GLU:HG3	3:o:100(D):ALA:HB2	1.88	0.56
3:o:189:LEU:HD23	3:o:189:LEU:N	2.21	0.55
4:v:81:GLU:CA	4:v:168:SER:O	2.54	0.55
1:S:193:SER:HB3	3:s:98:MET:SD	2.46	0.55
3:s:189:LEU:N	3:s:189:LEU:HD23	2.21	0.55
1:C:131:THR:OG1	3:c:100(H):ARG:NH2	2.40	0.55
1:G:212:THR:HG21	1:I:216:ASN:ND2	2.22	0.55
3:i:184:VAL:HG23	3:i:189:LEU:CD2	2.36	0.55
4:x:81:GLU:HA	4:x:168:SER:O	2.07	0.54
1:M:190:GLU:CD	3:m:100(D):ALA:HB2	2.32	0.54
1:S:136:SER:OG	3:s:100(E):GLY:O	2.17	0.54
1:E:226:LEU:HD21	3:e:100(E):GLY:HA3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:189:GLN:HG3	3:u:27(C):GLY:O	2.06	0.54
4:l:80:PRO:C	4:l:168:SER:O	2.51	0.54
4:r:40:PRO:HB3	4:r:165:GLU:HG3	1.89	0.54
3:s:184:VAL:CG2	3:s:189:LEU:HD21	2.38	0.54
4:f:40:PRO:CB	4:f:165:GLU:HG3	2.37	0.54
4:p:140:TYR:CG	4:p:141:PRO:HA	2.42	0.54
1:O:189:GLN:NE2	3:o:27(D):GLU:O	2.41	0.53
3:i:184:VAL:CG2	3:i:189:LEU:CD2	2.86	0.53
1:A:190:GLU:CD	3:a:100(D):ALA:CB	2.81	0.53
1:C:214:ILE:HD11	1:E:216:ASN:HD21	1.73	0.53
1:S:226:LEU:CD2	3:s:100(D):ALA:C	2.82	0.53
1:A:189:GLN:CG	3:a:27(C):GLY:O	2.56	0.53
4:p:185:ASP:O	4:p:186:TYR:C	2.50	0.53
4:d:106:ILE:HB	4:d:171:SER:HB3	1.89	0.53
3:e:189:LEU:HD23	3:e:189:LEU:N	2.22	0.53
3:i:11:LEU:HB2	3:i:147:PRO:HG3	1.89	0.53
4:j:90:GLN:OE1	4:j:92:ASP:N	2.42	0.53
3:c:184:VAL:HG23	3:c:189:LEU:HD21	1.90	0.53
3:s:184:VAL:CG2	3:s:189:LEU:CD2	2.87	0.53
3:q:184:VAL:HB	3:q:189:LEU:HD21	1.90	0.52
1:M:21:PRO:HA	2:N:15:GLU:OE2	2.10	0.52
3:c:184:VAL:CG2	3:c:189:LEU:CD2	2.88	0.52
3:g:184:VAL:CB	3:g:189:LEU:HD21	2.39	0.52
3:k:184:VAL:CG2	3:k:189:LEU:CD2	2.87	0.52
3:o:184:VAL:HG23	3:o:189:LEU:CD1	2.39	0.52
4:n:150:VAL:HG13	4:n:192:TYR:CE1	2.45	0.52
4:r:81:GLU:HA	4:r:168:SER:O	2.09	0.52
1:Q:222:TRP:CE2	1:Q:225:GLY:HA2	2.44	0.52
4:d:81:GLU:N	4:d:168:SER:O	2.42	0.52
3:c:184:VAL:HG23	3:c:189:LEU:CD2	2.40	0.52
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.44	0.52
1:U:325:GLU:O	1:U:326:LYS:C	2.53	0.52
1:I:222:TRP:CE2	1:I:225:GLY:HA2	2.44	0.52
3:k:184:VAL:HB	3:k:189:LEU:HD21	1.92	0.52
4:d:40:PRO:CB	4:d:165:GLU:HG3	2.40	0.52
3:s:184:VAL:HB	3:s:189:LEU:HD21	1.90	0.52
1:I:131:THR:OG1	3:i:100(H):ARG:NH2	2.42	0.51
1:S:222:TRP:CZ2	1:S:225:GLY:HA2	2.46	0.51
4:r:83:VAL:CG2	4:r:168:SER:HA	2.40	0.51
1:O:222:TRP:CZ2	1:O:225:GLY:HA2	2.44	0.51
1:U:205:SER:OG	1:W:221:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:185:PRO:O	3:k:189:LEU:HG	2.09	0.51
4:t:40:PRO:CB	4:t:165:GLU:HG3	2.41	0.51
1:Q:48:THR:CB	4:t:126:LYS:HD3	2.40	0.51
1:Q:185:PRO:HB3	1:Q:190:GLU:CD	2.35	0.51
4:n:40:PRO:HB3	4:n:165:GLU:HG3	1.93	0.51
3:o:184:VAL:CG2	3:o:189:LEU:CD2	2.89	0.51
4:p:81:GLU:HA	4:p:168:SER:O	2.10	0.51
3:s:184:VAL:HG23	3:s:189:LEU:HD21	1.92	0.51
3:w:97:SER:OG	3:w:100(N):ASP:OD2	2.20	0.51
1:K:136:SER:OG	3:k:100(E):GLY:O	2.28	0.51
3:a:184:VAL:CG2	3:a:189:LEU:CD2	2.88	0.51
3:o:184:VAL:HB	3:o:189:LEU:HD21	1.93	0.51
3:q:184:VAL:CG2	3:q:189:LEU:CD2	2.88	0.51
4:t:40:PRO:HB3	4:t:165:GLU:HG3	1.92	0.51
1:Q:189:GLN:CG	3:q:27(C):GLY:O	2.59	0.51
3:k:184:VAL:HG23	3:k:189:LEU:HD11	1.92	0.51
3:m:136:ALA:HB3	3:m:189:LEU:HD11	1.93	0.51
1:A:226:LEU:HD22	3:a:100(E):GLY:CA	2.41	0.51
4:l:83:VAL:HG22	4:l:168:SER:HA	1.93	0.51
4:r:40:PRO:CB	4:r:165:GLU:HG3	2.41	0.51
3:u:184:VAL:CG2	3:u:189:LEU:CD2	2.89	0.51
1:I:190:GLU:HG3	3:i:100(A):VAL:HG11	1.94	0.50
3:g:185:PRO:O	3:g:189:LEU:HG	2.11	0.50
4:v:125:LEU:C	4:v:127:SER:N	2.68	0.50
1:A:193:SER:HB3	3:a:98:MET:SD	2.51	0.50
1:I:190:GLU:CD	3:i:100(D):ALA:CB	2.84	0.50
3:o:185:PRO:O	3:o:189:LEU:HG	2.11	0.50
1:A:190:GLU:OE1	3:a:100(D):ALA:HB2	2.11	0.50
1:O:192:THR:OG1	3:o:27(C):GLY:HA2	2.11	0.50
1:O:226:LEU:HD21	3:o:100(E):GLY:CA	2.41	0.50
3:u:184:VAL:HG23	3:u:189:LEU:CD1	2.41	0.50
1:O:133:ASN:O	3:o:100(I):ALA:HB2	2.12	0.50
3:e:184:VAL:CG2	3:e:189:LEU:CD2	2.89	0.50
3:w:184:VAL:CG2	3:w:189:LEU:CD2	2.89	0.50
4:n:33:LEU:HD22	4:n:71:PHE:CG	2.47	0.50
4:b:40:PRO:CB	4:b:165:GLU:HG3	2.42	0.50
3:o:184:VAL:CG2	3:o:189:LEU:HD22	2.42	0.50
4:t:90:GLN:OE1	4:t:92:ASP:N	2.44	0.50
1:E:226:LEU:CD2	3:e:100(E):GLY:CA	2.89	0.50
4:x:140:TYR:CG	4:x:141:PRO:HA	2.47	0.50
1:K:222:TRP:CZ2	1:K:225:GLY:HA2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:184:VAL:HB	3:e:189:LEU:HD21	1.94	0.50
4:v:150:VAL:HG13	4:v:192:TYR:CE1	2.46	0.50
1:I:201:ARG:HD2	1:K:216:ASN:OD1	2.12	0.49
3:g:11:LEU:HD23	3:g:116:THR:HB	1.93	0.49
3:o:184:VAL:HB	3:o:189:LEU:CD2	2.41	0.49
4:p:81:GLU:CA	4:p:168:SER:O	2.60	0.49
4:h:33:LEU:HD22	4:h:71:PHE:CG	2.47	0.49
3:k:184:VAL:HG23	3:k:189:LEU:CD2	2.42	0.49
3:o:108:MET:HB3	3:o:149:PRO:HD3	1.94	0.49
3:u:185:PRO:O	3:u:189:LEU:HG	2.12	0.49
4:v:33:LEU:HD22	4:v:71:PHE:CG	2.47	0.49
1:O:205:SER:OG	1:Q:221:PRO:HD3	2.12	0.49
1:C:205:SER:OG	1:E:221:PRO:HD3	2.12	0.49
3:s:184:VAL:CB	3:s:189:LEU:HD21	2.43	0.49
4:t:83:VAL:CG2	4:t:168:SER:HA	2.42	0.49
1:I:189:GLN:CB	3:i:27(C):GLY:O	2.60	0.49
3:i:184:VAL:CG2	3:i:189:LEU:HD22	2.43	0.49
4:v:81:GLU:HA	4:v:168:SER:O	2.13	0.49
1:A:185:PRO:HB3	1:A:190:GLU:CD	2.38	0.49
3:a:184:VAL:HG23	3:a:189:LEU:CD2	2.43	0.49
4:b:12:SER:HB3	4:b:107:LYS:HE3	1.95	0.49
3:w:108:MET:HB3	3:w:149:PRO:HD3	1.94	0.49
1:O:98:TYR:OH	3:o:100(D):ALA:O	2.12	0.49
4:d:81:GLU:CA	4:d:168:SER:O	2.60	0.49
3:i:189:LEU:N	3:i:189:LEU:HD23	2.26	0.49
3:o:136:ALA:HB3	3:o:189:LEU:HD11	1.95	0.49
3:u:184:VAL:HB	3:u:189:LEU:HD21	1.93	0.49
4:l:106:ILE:HB	4:l:171:SER:HB3	1.94	0.49
3:m:184:VAL:CG2	3:m:189:LEU:CD2	2.90	0.49
1:U:226:LEU:HD21	3:u:100(E):GLY:CA	2.43	0.49
1:O:201:ARG:HD2	1:Q:216:ASN:OD1	2.13	0.48
4:b:33:LEU:HD22	4:b:71:PHE:CG	2.47	0.48
1:E:190:GLU:CD	3:e:100(D):ALA:CB	2.84	0.48
4:d:50:ASP:OD1	4:d:91:TYR:OH	2.13	0.48
3:g:184:VAL:HB	3:g:189:LEU:HD21	1.94	0.48
4:j:108:ARG:NH2	4:j:111:ALA:HB2	2.29	0.48
1:W:226:LEU:HD21	3:w:100(E):GLY:CA	2.44	0.48
4:h:81:GLU:HA	4:h:168:SER:O	2.14	0.48
4:r:33:LEU:HD22	4:r:71:PHE:CG	2.47	0.48
4:f:33:LEU:HD22	4:f:71:PHE:CG	2.48	0.48
1:I:205:SER:OG	1:K:221:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:LEU:CD1	3:i:100(E):GLY:HA3	2.44	0.48
3:i:184:VAL:CG2	3:i:189:LEU:HD21	2.44	0.48
3:k:184:VAL:CB	3:k:189:LEU:HD21	2.44	0.48
3:u:184:VAL:HB	3:u:189:LEU:CD2	2.44	0.48
3:u:136:ALA:HB3	3:u:189:LEU:HD11	1.96	0.48
4:p:33:LEU:HD22	4:p:71:PHE:CG	2.48	0.47
4:p:108:ARG:HD3	4:p:140:TYR:CG	2.49	0.47
1:K:226:LEU:HD21	3:k:100(E):GLY:N	2.28	0.47
4:f:50:ASP:OD1	4:f:91:TYR:OH	2.17	0.47
3:i:27(C):GLY:O	3:i:27(D):GLU:HB2	2.14	0.47
3:k:97:SER:OG	3:k:100(N):ASP:OD2	2.19	0.47
3:q:184:VAL:HG23	3:q:189:LEU:CD1	2.44	0.47
4:v:40:PRO:CG	4:v:165:GLU:HG3	2.44	0.47
3:c:184:VAL:CG2	3:c:189:LEU:HD21	2.45	0.47
3:u:11:LEU:HD21	3:u:114:ALA:O	2.14	0.47
3:u:184:VAL:HG23	3:u:189:LEU:CD2	2.44	0.47
3:a:11:LEU:HB2	3:a:147:PRO:HG3	1.97	0.47
4:p:150:VAL:HG13	4:p:192:TYR:CE1	2.49	0.47
1:K:189:GLN:CD	3:k:27(C):GLY:O	2.58	0.47
1:W:133:ASN:O	3:w:100(I):ALA:HB2	2.15	0.47
3:g:182:VAL:HG22	3:g:184:VAL:HG13	1.96	0.47
3:k:182:VAL:HG22	3:k:184:VAL:HG13	1.97	0.47
3:q:97:SER:OG	3:q:100(N):ASP:OD2	2.32	0.47
3:q:184:VAL:CB	3:q:189:LEU:HD21	2.45	0.47
4:x:90:GLN:CD	4:x:90:GLN:C	2.83	0.47
1:A:137:ASN:ND2	3:a:100(G):GLU:OE1	2.47	0.47
1:E:185:PRO:HB3	1:E:190:GLU:CD	2.39	0.47
4:p:108:ARG:NE	4:p:109:THR:O	2.46	0.47
3:q:13:GLN:NE2	3:q:113:SER:O	2.48	0.47
3:m:13:GLN:NE2	3:m:113:SER:O	2.47	0.47
3:m:184:VAL:HB	3:m:189:LEU:HD21	1.97	0.47
4:t:81:GLU:HA	4:t:168:SER:O	2.14	0.47
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.50	0.47
3:k:184:VAL:HB	3:k:189:LEU:CD2	2.45	0.47
4:x:150:VAL:HG13	4:x:192:TYR:CE1	2.50	0.47
1:I:225:GLY:C	1:I:226:LEU:HD23	2.40	0.46
4:p:81:GLU:N	4:p:168:SER:O	2.48	0.46
4:v:108:ARG:NE	4:v:109:THR:O	2.39	0.46
1:M:222:TRP:CZ2	1:M:225:GLY:HA2	2.50	0.46
3:e:184:VAL:CG2	3:e:189:LEU:HD22	2.45	0.46
4:l:150:VAL:HG13	4:l:192:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:12:SER:CB	4:n:107:LYS:HE3	2.44	0.46
4:t:33:LEU:HD22	4:t:71:PHE:CG	2.49	0.46
1:A:226:LEU:HD22	3:a:100(E):GLY:HA3	1.93	0.46
1:G:189:GLN:HG3	3:g:27(C):GLY:O	2.15	0.46
1:I:189:GLN:CG	3:i:27(C):GLY:O	2.61	0.46
3:a:184:VAL:CG2	3:a:189:LEU:HD22	2.45	0.46
4:b:30:ARG:HD2	4:b:30:ARG:N	2.31	0.46
4:h:81:GLU:N	4:h:168:SER:O	2.48	0.46
3:u:108:MET:CB	3:u:149:PRO:HD3	2.44	0.46
1:A:189:GLN:HG3	3:a:27(C):GLY:O	2.16	0.46
4:f:90:GLN:OE1	4:f:92:ASP:N	2.48	0.46
4:j:11:LEU:HD21	4:j:19:VAL:HG13	1.97	0.46
3:m:184:VAL:HG23	3:m:189:LEU:CD2	2.46	0.46
1:I:194:LEU:HD21	3:i:100(F):TRP:CD2	2.50	0.46
1:K:222:TRP:CE2	1:K:225:GLY:HA2	2.50	0.46
1:Q:207[B]:ARG:NH1	1:Q:240:GLY:O	2.48	0.46
3:e:95:HIS:CE1	3:e:100(P):PHE:CE2	3.04	0.46
3:o:184:VAL:HG23	3:o:189:LEU:CD2	2.45	0.46
1:M:226:LEU:HD21	3:m:100(D):ALA:C	2.40	0.46
1:Q:194:LEU:HD21	3:q:100(F):TRP:CD2	2.51	0.46
4:b:150:VAL:HG13	4:b:192:TYR:CE1	2.51	0.46
4:f:187:GLU:O	4:f:211:ARG:NH2	2.49	0.46
1:G:324:PRO:C	1:G:325:GLU:HG2	2.41	0.46
1:M:21:PRO:O	1:M:324:PRO:HG3	2.16	0.46
1:O:226:LEU:HD21	3:o:100(E):GLY:HA2	1.97	0.46
3:c:184:VAL:CG2	3:c:189:LEU:HD22	2.46	0.46
4:f:40:PRO:HB2	4:f:165:GLU:HG3	1.96	0.46
4:v:11:LEU:HD21	4:v:19:VAL:HG13	1.98	0.46
1:I:186:SER:OG	3:i:100(C):SER:HB2	2.15	0.46
3:g:116:THR:OG1	3:g:147:PRO:HD3	2.16	0.46
3:u:182:VAL:HG22	3:u:184:VAL:HG13	1.98	0.46
3:w:184:VAL:HB	3:w:189:LEU:HD21	1.98	0.46
4:x:108:ARG:NH1	4:x:172:THR:HG22	2.30	0.46
1:C:190:GLU:HG3	3:c:100(D):ALA:HB2	1.97	0.46
1:O:226:LEU:CD2	3:o:100(E):GLY:CA	2.94	0.46
3:w:95:HIS:CE1	3:w:100(P):PHE:CE2	3.04	0.46
4:b:23:CYS:HB2	4:b:35:TRP:CH2	2.52	0.45
3:i:186:SER:HA	3:i:189:LEU:HG	1.97	0.45
3:m:178:LEU:HD23	3:m:178:LEU:C	2.41	0.45
3:s:184:VAL:HG23	3:s:189:LEU:CD2	2.46	0.45
1:A:206:THR:C	1:C:221:PRO:HG2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:80:PRO:C	4:b:168:SER:O	2.58	0.45
4:d:80:PRO:C	4:d:168:SER:O	2.59	0.45
3:e:184:VAL:HB	3:e:189:LEU:CD2	2.46	0.45
4:j:90:GLN:C	4:j:90:GLN:CD	2.84	0.45
3:u:184:VAL:CB	3:u:189:LEU:HD21	2.46	0.45
1:G:190:GLU:CG	3:g:100(D):ALA:HB2	2.46	0.45
1:I:153:TRP:CD1	1:I:252:ILE:CD1	3.00	0.45
1:U:136:SER:CB	3:u:100(E):GLY:O	2.65	0.45
4:d:90:GLN:C	4:d:90:GLN:CD	2.83	0.45
3:s:136:ALA:HB3	3:s:189:LEU:HD11	1.98	0.45
4:v:40:PRO:HG2	4:v:165:GLU:HG3	1.98	0.45
4:v:90:GLN:CD	4:v:90:GLN:C	2.85	0.45
4:l:11:LEU:HD21	4:l:19:VAL:HG13	1.98	0.45
4:r:90:GLN:C	4:r:90:GLN:CD	2.85	0.45
3:w:184:VAL:HG23	3:w:189:LEU:CD2	2.46	0.45
1:W:193:SER:HB3	3:w:98:MET:SD	2.57	0.45
4:l:81:GLU:CA	4:l:168:SER:O	2.65	0.45
3:o:11:LEU:HD21	3:o:114:ALA:O	2.17	0.45
4:r:83:VAL:HG22	4:r:168:SER:HA	1.98	0.45
1:C:226:LEU:HD21	3:c:100(E):GLY:CA	2.46	0.45
1:O:222:TRP:CE2	1:O:225:GLY:HA2	2.52	0.45
3:e:145:TYR:CE2	3:e:150:VAL:HG13	2.51	0.45
3:e:178:LEU:C	3:e:178:LEU:HD23	2.41	0.45
3:q:184:VAL:HB	3:q:189:LEU:CD2	2.45	0.45
4:t:108:ARG:NH2	4:t:111:ALA:HB2	2.32	0.45
3:u:184:VAL:CG2	3:u:189:LEU:HD22	2.47	0.45
4:x:108:ARG:NH2	4:x:111:ALA:HB2	2.31	0.45
2:D:17[A]:MET:HE1	2:D:23:GLY:HA3	1.99	0.45
4:v:80:PRO:C	4:v:168:SER:O	2.60	0.45
1:I:194:LEU:CD2	3:i:100(F):TRP:CD2	2.99	0.45
3:c:97:SER:OG	3:c:100(N):ASP:OD2	2.31	0.45
4:r:80:PRO:HB2	4:r:169:LYS:O	2.17	0.45
4:x:90:GLN:OE1	4:x:92:ASP:N	2.49	0.45
1:C:136:SER:CB	3:c:100(E):GLY:O	2.65	0.45
4:d:140:TYR:CG	4:d:141:PRO:HA	2.51	0.45
3:a:184:VAL:HB	3:a:189:LEU:HD21	1.99	0.45
4:l:90:GLN:OE1	4:l:92:ASP:N	2.49	0.45
3:q:185:PRO:O	3:q:189:LEU:HG	2.17	0.45
3:w:145:TYR:CE2	3:w:150:VAL:HG13	2.51	0.45
4:d:141:PRO:HG3	4:d:199:GLN:NE2	2.32	0.44
3:e:185:PRO:O	3:e:189:LEU:HG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:11:LEU:HD21	3:i:114:ALA:O	2.17	0.44
3:o:184:VAL:CB	3:o:189:LEU:HD21	2.47	0.44
4:r:108:ARG:NH2	4:r:111:ALA:HB2	2.32	0.44
1:Q:48:THR:HB	4:t:126:LYS:HD3	1.99	0.44
1:U:226:LEU:HD21	3:u:100(E):GLY:HA3	1.99	0.44
3:q:178:LEU:C	3:q:178:LEU:HD23	2.42	0.44
3:q:184:VAL:HG23	3:q:189:LEU:CD2	2.47	0.44
4:v:125:LEU:C	4:v:127:SER:H	2.25	0.44
1:K:193:SER:HB3	3:k:98:MET:SD	2.56	0.44
4:f:90:GLN:C	4:f:90:GLN:CD	2.86	0.44
3:i:97:SER:OG	3:i:100(N):ASP:OD2	2.32	0.44
4:p:90:GLN:C	4:p:90:GLN:CD	2.85	0.44
1:G:190:GLU:HG3	3:g:100(D):ALA:HB2	2.00	0.44
1:G:304:ALA:HA	2:H:61:GLU:HA	2.00	0.44
1:I:225:GLY:O	1:I:226:LEU:HD23	2.17	0.44
3:a:184:VAL:HG23	3:a:189:LEU:HD21	1.98	0.44
4:x:33:LEU:HD22	4:x:71:PHE:CG	2.52	0.44
1:A:133:ASN:O	3:a:100(I):ALA:HB2	2.18	0.44
1:Q:225:GLY:C	1:Q:226:LEU:HD23	2.42	0.44
4:j:187:GLU:O	4:j:211:ARG:NH2	2.51	0.44
3:q:95:HIS:CE1	3:q:100(P):PHE:CE2	3.05	0.44
4:r:150:VAL:HG13	4:r:192:TYR:CE1	2.52	0.44
3:s:108:MET:HG2	3:s:149:PRO:HD3	2.00	0.44
4:v:90:GLN:OE1	4:v:92:ASP:N	2.50	0.44
3:w:184:VAL:HG23	3:w:189:LEU:HD21	1.99	0.44
1:C:201:ARG:HD2	1:E:216:ASN:OD1	2.17	0.44
1:I:194:LEU:CD2	3:i:100(F):TRP:CE3	3.00	0.44
1:Q:226:LEU:HD22	3:q:100(E):GLY:CA	2.43	0.44
4:d:125:LEU:C	4:d:127:SER:N	2.74	0.44
4:h:90:GLN:C	4:h:90:GLN:CD	2.86	0.44
4:p:108:ARG:HD3	4:p:140:TYR:CD1	2.53	0.44
3:u:108:MET:HB3	3:u:149:PRO:HD3	1.98	0.44
3:w:11:LEU:HD21	3:w:114:ALA:O	2.18	0.44
1:A:189:GLN:NE2	3:a:27(E):SER:HA	2.32	0.44
1:A:216:ASN:ND2	1:E:212:THR:CG2	2.80	0.44
4:n:90:GLN:C	4:n:90:GLN:CD	2.86	0.44
4:p:108:ARG:NH1	4:p:172:THR:HG22	2.32	0.44
4:r:11:LEU:HD21	4:r:19:VAL:HG13	2.00	0.44
4:t:150:VAL:HG13	4:t:192:TYR:CE1	2.52	0.44
1:O:192:THR:OG1	3:o:27(C):GLY:CA	2.66	0.44
4:b:11:LEU:HD21	4:b:19:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:33:LEU:HD22	4:d:71:PHE:CG	2.53	0.44
4:x:11:LEU:HD21	4:x:19:VAL:HG13	1.99	0.44
1:G:216:ASN:OD1	1:K:212:THR:HG21	2.18	0.43
4:b:81:GLU:HA	4:b:168:SER:O	2.18	0.43
4:l:81:GLU:N	4:l:168:SER:O	2.51	0.43
3:m:185:PRO:O	3:m:189:LEU:HG	2.18	0.43
4:n:187:GLU:O	4:n:211:ARG:NH2	2.51	0.43
4:p:39:LYS:NZ	4:p:168:SER:OG	2.48	0.43
3:q:145:TYR:CE2	3:q:150:VAL:HG13	2.53	0.43
3:q:182:VAL:HG22	3:q:184:VAL:HG13	2.00	0.43
3:q:184:VAL:HG23	3:q:189:LEU:HD11	2.01	0.43
1:G:221:PRO:HD3	1:K:205:SER:OG	2.17	0.43
2:J:142:HIS:HB2	2:J:165:GLU:CD	2.43	0.43
2:P:142:HIS:HB2	2:P:165:GLU:CD	2.43	0.43
3:a:13:GLN:NE2	3:a:113:SER:O	2.50	0.43
3:e:184:VAL:HG23	3:e:189:LEU:CD2	2.47	0.43
4:f:11:LEU:HD21	4:f:19:VAL:HG13	2.00	0.43
3:k:128:SER:O	3:k:129:LYS:HB3	2.17	0.43
4:p:11:LEU:HD21	4:p:19:VAL:HG13	2.00	0.43
4:h:11:LEU:HD21	4:h:19:VAL:HG13	1.99	0.43
3:k:184:VAL:CG2	3:k:189:LEU:HD22	2.49	0.43
4:l:12:SER:CB	4:l:107:LYS:HE3	2.45	0.43
4:v:140:TYR:CG	4:v:141:PRO:HA	2.53	0.43
1:A:189:GLN:HG3	3:a:27(C):GLY:HA3	2.01	0.43
2:H:142:HIS:HB2	2:H:165:GLU:CD	2.43	0.43
4:l:90:GLN:CD	4:l:90:GLN:C	2.86	0.43
2:R:142:HIS:HB2	2:R:165:GLU:CD	2.43	0.43
3:k:100:GLN:HB2	3:k:100(G):GLU:HG2	2.01	0.43
4:v:30:ARG:HD2	4:v:30:ARG:N	2.34	0.43
3:w:184:VAL:CG2	3:w:189:LEU:HD22	2.48	0.43
1:Q:15:LEU:HD11	2:R:24:PHE:CE2	2.54	0.43
3:e:184:VAL:CB	3:e:189:LEU:HD21	2.48	0.43
4:t:123:GLU:HA	4:t:126:LYS:HE3	2.00	0.43
1:G:102:VAL:HG22	1:G:232:ILE:HB	2.00	0.43
1:M:212:THR:HG21	1:O:216:ASN:OD1	2.19	0.43
3:e:184:VAL:HG23	3:e:189:LEU:CD1	2.49	0.43
4:l:40:PRO:CB	4:l:165:GLU:HG3	2.49	0.43
1:U:190:GLU:HG3	3:u:100(D):ALA:HB2	2.00	0.43
4:d:181:LEU:CD1	4:d:186:TYR:HB2	2.49	0.43
3:k:184:VAL:HG23	3:k:189:LEU:HD21	2.01	0.43
4:n:11:LEU:HD21	4:n:19:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:178:LEU:C	3:o:178:LEU:HD23	2.43	0.43
3:e:128:SER:O	3:e:129:LYS:HB3	2.19	0.43
3:m:184:VAL:HG23	3:m:189:LEU:HD21	2.01	0.43
3:q:184:VAL:CG2	3:q:189:LEU:HD22	2.49	0.43
3:w:184:VAL:CG2	3:w:189:LEU:HD21	2.49	0.43
1:I:111:LEU:HB2	2:L:73:VAL:HG11	2.00	0.43
1:M:212:THR:CG2	1:O:216:ASN:ND2	2.81	0.43
4:j:40:PRO:HB3	4:j:165:GLU:HG3	2.00	0.43
3:m:184:VAL:CG2	3:m:189:LEU:HD22	2.49	0.43
4:t:90:GLN:C	4:t:90:GLN:CD	2.86	0.43
3:u:4:LEU:HD13	3:u:92:CYS:SG	2.59	0.43
4:v:11:LEU:HD12	4:v:11:LEU:C	2.44	0.43
1:I:214:ILE:HD11	1:K:216:ASN:ND2	2.32	0.42
1:Q:189:GLN:NE2	3:q:27(E):SER:HA	2.34	0.42
3:a:178:LEU:HD23	3:a:178:LEU:C	2.44	0.42
4:b:90:GLN:CD	4:b:90:GLN:C	2.86	0.42
4:j:125:LEU:C	4:j:127:SER:N	2.73	0.42
3:u:13:GLN:NE2	3:u:113:SER:O	2.52	0.42
1:I:186:SER:OG	3:i:100(C):SER:O	2.32	0.42
1:K:136:SER:CB	3:k:100(E):GLY:O	2.67	0.42
1:M:216:ASN:ND2	1:Q:212:THR:CG2	2.82	0.42
1:W:155:THR:HG21	3:w:100(F):TRP:NE1	2.34	0.42
3:g:189:LEU:HD22	3:g:194:TYR:CE2	2.53	0.42
4:j:33:LEU:HD22	4:j:71:PHE:CG	2.54	0.42
3:q:136:ALA:HB3	3:q:189:LEU:HD11	2.01	0.42
3:s:128:SER:O	3:s:129:LYS:HB3	2.19	0.42
3:w:185:PRO:O	3:w:189:LEU:CD2	2.67	0.42
3:a:128:SER:O	3:a:129:LYS:HB3	2.19	0.42
3:g:178:LEU:C	3:g:178:LEU:HD23	2.44	0.42
3:q:184:VAL:CG2	3:q:189:LEU:HD21	2.49	0.42
1:K:226:LEU:CD2	3:k:100(E):GLY:N	2.82	0.42
1:O:305:CYS:O	2:P:60:ASN:ND2	2.52	0.42
1:W:207[B]:ARG:NH1	1:W:240:GLY:O	2.50	0.42
1:W:273:PRO:HB3	4:f:24:GLN:OE1	2.19	0.42
4:j:23:CYS:HB2	4:j:35:TRP:CH2	2.54	0.42
3:k:178:LEU:C	3:k:178:LEU:HD23	2.44	0.42
1:G:131:THR:HG21	3:g:100(H):ARG:HG3	2.01	0.42
4:b:11:LEU:HD12	4:b:11:LEU:C	2.43	0.42
4:d:40:PRO:CG	4:d:165:GLU:HG3	2.49	0.42
4:h:90:GLN:OE1	4:h:92:ASP:N	2.53	0.42
3:m:128:SER:O	3:m:129:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:LEU:CD2	3:e:100(F):TRP:CD2	3.02	0.42
1:I:184:HIS:O	1:I:228[B]:SER:HB3	2.20	0.42
1:U:222:TRP:CZ2	1:U:225:GLY:HA2	2.54	0.42
3:a:184:VAL:CG2	3:a:189:LEU:HD21	2.49	0.42
4:h:80:PRO:C	4:h:168:SER:O	2.63	0.42
3:k:184:VAL:CG2	3:k:189:LEU:HD21	2.50	0.42
4:l:11:LEU:HD12	4:l:11:LEU:C	2.44	0.42
1:O:49:GLY:HA2	1:O:285:ASN:O	2.19	0.42
1:S:212:THR:CG2	1:U:216:ASN:ND2	2.82	0.42
3:c:95:HIS:CE1	3:c:100(P):PHE:CE2	3.07	0.42
3:g:192:GLN:NE2	3:g:194:TYR:OH	2.53	0.42
3:i:31:TYR:CE1	3:i:100(A):VAL:HG13	2.55	0.42
4:p:196:VAL:O	4:p:204:PRO:HA	2.20	0.42
3:w:128:SER:O	3:w:129:LYS:HB3	2.20	0.42
4:n:11:LEU:HD12	4:n:11:LEU:C	2.44	0.42
4:t:140:TYR:CG	4:t:141:PRO:HA	2.55	0.42
4:x:30:ARG:HD2	4:x:30:ARG:N	2.35	0.42
1:M:221:PRO:HD3	1:Q:205:SER:OG	2.20	0.42
4:d:11:LEU:HD21	4:d:19:VAL:HG13	2.01	0.42
4:d:90:GLN:OE1	4:d:92:ASP:N	2.53	0.42
4:h:11:LEU:C	4:h:11:LEU:HD12	2.44	0.42
4:j:140:TYR:CG	4:j:141:PRO:HA	2.54	0.42
3:m:184:VAL:CG2	3:m:189:LEU:HD21	2.50	0.42
4:t:30:ARG:N	4:t:30:ARG:HD2	2.35	0.42
3:u:95:HIS:CE1	3:u:100(P):PHE:CE2	3.08	0.42
3:i:128:SER:O	3:i:129:LYS:HB3	2.20	0.42
3:i:145:TYR:CE2	3:i:150:VAL:HG13	2.55	0.42
3:k:11:LEU:HB2	3:k:147:PRO:HG3	2.00	0.42
1:O:111:LEU:HB2	2:R:73:VAL:HG11	2.01	0.41
1:S:216:ASN:ND2	1:W:212:THR:CG2	2.82	0.41
4:l:188:LYS:HB3	4:l:189:HIS:CD2	2.55	0.41
3:e:185:PRO:O	3:e:189:LEU:CD2	2.68	0.41
3:g:128:SER:O	3:g:129:LYS:HB3	2.21	0.41
4:j:125:LEU:C	4:j:127:SER:H	2.28	0.41
3:k:145:TYR:CE2	3:k:150:VAL:HG13	2.55	0.41
3:q:128:SER:O	3:q:129:LYS:HB3	2.20	0.41
1:I:133:ASN:O	3:i:100(I):ALA:CB	2.67	0.41
3:a:4:LEU:HD13	3:a:92:CYS:SG	2.60	0.41
3:q:184:VAL:HG23	3:q:189:LEU:HD21	2.02	0.41
4:d:11:LEU:HD12	4:d:11:LEU:C	2.44	0.41
4:l:80:PRO:HB2	4:l:169:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:GLU:CG	3:c:100(D):ALA:HB2	2.51	0.41
1:S:167:THR:HB	5:EA:1:NAG:H62	2.02	0.41
1:S:212:THR:HG21	1:U:216:ASN:OD1	2.20	0.41
2:X:60:ASN:O	2:X:60:ASN:ND2	2.54	0.41
4:h:188:LYS:HB3	4:h:189:HIS:CD2	2.55	0.41
1:A:212:THR:CG2	1:C:216:ASN:ND2	2.83	0.41
1:O:190:GLU:OE2	3:o:100(D):ALA:HA	2.20	0.41
1:S:205:SER:OG	1:U:221:PRO:HD3	2.20	0.41
1:U:111:LEU:HB2	2:X:73:VAL:HG11	2.02	0.41
1:U:214:ILE:HD11	1:W:216:ASN:ND2	2.34	0.41
3:c:100(O):ALA:HB2	4:d:34:ASN:CG	2.45	0.41
3:s:178:LEU:C	3:s:178:LEU:HD23	2.45	0.41
3:s:185:PRO:O	3:s:189:LEU:HG	2.20	0.41
2:B:18:ILE:HB	1:K:275[B]:ASP:OD1	2.21	0.41
1:I:190:GLU:OE2	3:i:100(D):ALA:CB	2.68	0.41
2:N:60:ASN:O	2:N:60:ASN:ND2	2.54	0.41
1:S:185:PRO:HB3	1:S:190:GLU:CD	2.45	0.41
1:U:207[B]:ARG:NH1	1:U:240:GLY:O	2.51	0.41
4:h:140:TYR:CG	4:h:141:PRO:HA	2.56	0.41
3:s:184:VAL:HG23	3:s:189:LEU:HD11	2.01	0.41
4:t:181:LEU:CD1	4:t:186:TYR:HB2	2.50	0.41
3:u:185:PRO:O	3:u:189:LEU:CD2	2.69	0.41
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.55	0.41
1:C:260[B]:MET:HE1	2:F:73:VAL:HG21	2.01	0.41
1:E:189:GLN:CG	3:e:27(C):GLY:O	2.62	0.41
1:I:228[B]:SER:OG	3:i:100(D):ALA:CB	2.68	0.41
2:V:17[A]:MET:HE1	2:V:23:GLY:HA3	2.02	0.41
1:W:92:LYS:HD3	4:f:27:GLN:HB2	2.02	0.41
3:c:128:SER:O	3:c:129:LYS:HB3	2.21	0.41
3:u:11:LEU:HD23	3:u:116:THR:N	2.35	0.41
3:u:128:SER:O	3:u:129:LYS:HB3	2.21	0.41
3:u:178:LEU:C	3:u:178:LEU:HD23	2.45	0.41
3:w:178:LEU:HD23	3:w:178:LEU:C	2.46	0.41
2:F:60:ASN:ND2	2:F:60:ASN:O	2.54	0.41
1:G:307:LYS:HD3	2:H:92:TRP:CE2	2.56	0.41
1:O:190:GLU:HB2	3:o:100(C):SER:OG	2.21	0.41
1:U:201:ARG:HD2	1:W:216:ASN:OD1	2.20	0.41
1:W:92:LYS:HD3	4:f:27:GLN:CB	2.51	0.41
3:a:184:VAL:CB	3:a:189:LEU:HD21	2.51	0.41
3:c:145:TYR:CE2	3:c:150:VAL:HG13	2.56	0.41
4:f:83:VAL:CG1	4:f:106:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:81:GLU:CA	4:h:168:SER:O	2.69	0.41
3:k:136:ALA:HB3	3:k:189:LEU:HD11	2.02	0.41
4:n:30:ARG:HD2	4:n:30:ARG:N	2.36	0.41
3:s:182:VAL:HG22	3:s:184:VAL:HG13	2.02	0.41
4:t:11:LEU:HD21	4:t:19:VAL:HG13	2.03	0.41
3:w:184:VAL:CB	3:w:189:LEU:HD21	2.51	0.41
1:I:190:GLU:HA	1:I:193:SER:HB2	2.02	0.41
1:W:273:PRO:CB	4:f:24:GLN:OE1	2.69	0.41
3:m:11:LEU:HD21	3:m:114:ALA:O	2.21	0.41
4:n:80:PRO:C	4:n:168:SER:O	2.64	0.41
4:p:108:ARG:NH2	4:p:109:THR:O	2.53	0.41
3:g:189:LEU:CD2	3:g:194:TYR:CE2	3.04	0.40
4:j:11:LEU:HD12	4:j:11:LEU:C	2.47	0.40
3:m:108:MET:HB3	3:m:149:PRO:HD3	2.03	0.40
3:m:145:TYR:CE2	3:m:150:VAL:HG13	2.56	0.40
3:o:95:HIS:CE1	3:o:100(P):PHE:CE2	3.09	0.40
3:w:108:MET:CB	3:w:149:PRO:HD3	2.51	0.40
1:S:226:LEU:HA	1:S:226:LEU:HD23	1.83	0.40
1:W:222:TRP:CZ2	1:W:225:GLY:HA2	2.56	0.40
4:f:108:ARG:NE	4:f:109:THR:O	2.51	0.40
3:o:185:PRO:O	3:o:189:LEU:CD2	2.69	0.40
4:p:141:PRO:HG3	4:p:199:GLN:NE2	2.37	0.40
4:r:140:TYR:CG	4:r:141:PRO:HA	2.57	0.40
3:w:184:VAL:HB	3:w:189:LEU:CD2	2.51	0.40
4:x:11:LEU:HD12	4:x:11:LEU:C	2.46	0.40
1:U:190:GLU:CD	3:u:100(D):ALA:HB2	2.46	0.40
3:g:4:LEU:HD13	3:g:92:CYS:SG	2.61	0.40
3:k:13:GLN:NE2	3:k:113:SER:O	2.54	0.40
3:k:123:PRO:HD2	4:l:121:SER:CB	2.51	0.40
4:n:110:VAL:HG13	4:n:140:TYR:O	2.22	0.40
4:r:83:VAL:CG1	4:r:106:ILE:HG12	2.52	0.40
1:C:16:GLY:HA3	2:D:14:TRP:CH2	2.56	0.40
1:I:190:GLU:OE2	1:I:194:LEU:HD11	2.21	0.40
2:R:17[A]:MET:HE1	2:R:23:GLY:HA3	2.04	0.40
4:h:40:PRO:HB3	4:h:165:GLU:HG3	2.02	0.40
4:h:150:VAL:HG13	4:h:192:TYR:CE1	2.57	0.40
4:r:11:LEU:HD12	4:r:11:LEU:C	2.46	0.40
4:t:11:LEU:HD12	4:t:11:LEU:C	2.47	0.40
4:t:80:PRO:HB2	4:t:169:LYS:O	2.21	0.40
1:G:205:SER:OG	1:I:221:PRO:HD3	2.21	0.40
1:O:276:THR:O	1:O:276:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:216:ASN:OD1	1:W:212:THR:HG21	2.20	0.40
2:V:142:HIS:HB2	2:V:165:GLU:CD	2.46	0.40
3:a:100(O):ALA:HB2	4:b:34:ASN:CG	2.46	0.40
4:d:125:LEU:C	4:d:127:SER:H	2.30	0.40
3:m:184:VAL:CB	3:m:189:LEU:HD21	2.51	0.40
3:s:13:GLN:NE2	3:s:113:SER:O	2.53	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:202:SER:OG	4:v:108:ARG:O[1_545]	1.78	0.42
4:h:202:SER:OG	4:n:108:ARG:O[1_564]	1.83	0.37
4:l:108:ARG:O	4:p:202:SER:OG[1_564]	1.87	0.33
1:U:312:ASN:ND2	4:h:187:GLU:OE2[1_646]	1.93	0.27
1:U:33:GLN:NE2	4:h:127:SER:O[1_646]	2.09	0.11
1:A:133:ASN:ND2	4:j:26:SER:O[1_545]	2.12	0.08
1:U:312:ASN:OD1	4:h:183:LYS:NZ[1_646]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	C	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	E	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	G	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	I	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	K	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	M	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	Q	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	S	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
1	U	328/323 (102%)	323 (98%)	4 (1%)	1 (0%)	36	70
1	W	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	36	70
2	B	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	D	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	F	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	H	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	J	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	L	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	N	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	P	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	R	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	T	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	V	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	X	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
3	a	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	c	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	e	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	g	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	i	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	k	241/241 (100%)	235 (98%)	6 (2%)	0	100	100
3	m	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	o	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	q	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	s	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	u	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	w	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
4	b	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	d	212/214 (99%)	209 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	f	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	h	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	j	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	l	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	n	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	p	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	r	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	t	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	v	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	x	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	11496/11424 (101%)	11268 (98%)	216 (2%)	12 (0%)	48	81

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
1	G	62	ILE
1	I	62	ILE
1	K	62	ILE
1	M	62	ILE
1	O	62	ILE
1	Q	62	ILE
1	S	62	ILE
1	U	62	ILE
1	W	62	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	C	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	E	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	G	291/283 (103%)	290 (100%)	1 (0%)	86	85
1	I	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	K	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	M	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	O	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	Q	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	S	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	U	291/283 (103%)	289 (99%)	2 (1%)	76	79
1	W	291/283 (103%)	289 (99%)	2 (1%)	76	79
2	B	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	D	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	F	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	H	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	J	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	L	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	N	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	P	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	R	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	T	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	V	153/148 (103%)	152 (99%)	1 (1%)	76	79
2	X	153/148 (103%)	152 (99%)	1 (1%)	76	79
3	a	202/200 (101%)	198 (98%)	4 (2%)	48	66
3	c	202/200 (101%)	197 (98%)	5 (2%)	42	62
3	e	202/200 (101%)	197 (98%)	5 (2%)	42	62
3	g	202/200 (101%)	198 (98%)	4 (2%)	48	66
3	i	202/200 (101%)	196 (97%)	6 (3%)	36	57
3	k	202/200 (101%)	197 (98%)	5 (2%)	42	62
3	m	202/200 (101%)	198 (98%)	4 (2%)	48	66
3	o	202/200 (101%)	197 (98%)	5 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	q	202/200 (101%)	198 (98%)	4 (2%)	48	66
3	s	202/200 (101%)	198 (98%)	4 (2%)	48	66
3	u	202/200 (101%)	197 (98%)	5 (2%)	42	62
3	w	202/200 (101%)	198 (98%)	4 (2%)	48	66
4	b	187/187 (100%)	179 (96%)	8 (4%)	26	49
4	d	187/187 (100%)	179 (96%)	8 (4%)	26	49
4	f	187/187 (100%)	178 (95%)	9 (5%)	23	46
4	h	187/187 (100%)	178 (95%)	9 (5%)	23	46
4	j	187/187 (100%)	180 (96%)	7 (4%)	30	52
4	l	187/187 (100%)	178 (95%)	9 (5%)	23	46
4	n	187/187 (100%)	179 (96%)	8 (4%)	26	49
4	p	187/187 (100%)	178 (95%)	9 (5%)	23	46
4	r	187/187 (100%)	178 (95%)	9 (5%)	23	46
4	t	187/187 (100%)	178 (95%)	9 (5%)	23	46
4	v	187/187 (100%)	178 (95%)	9 (5%)	23	46
4	x	187/187 (100%)	178 (95%)	9 (5%)	23	46
All	All	9996/9816 (102%)	9803 (98%)	193 (2%)	48	67

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	325	GLU
2	B	60	ASN
1	C	53	ASN
1	C	325	GLU
2	D	60	ASN
1	E	53	ASN
1	E	325	GLU
2	F	60	ASN
1	G	53	ASN
2	H	60	ASN
1	I	53	ASN
1	I	325	GLU
2	J	60	ASN
1	K	53	ASN

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Mol	Chain	Res	Type
1	K	325	GLU
2	L	60	ASN
1	M	53	ASN
1	M	325	GLU
2	N	60	ASN
1	O	53	ASN
1	O	325	GLU
2	P	60	ASN
1	Q	53	ASN
1	Q	325	GLU
2	R	60	ASN
1	S	53	ASN
1	S	325	GLU
2	T	60	ASN
1	U	53	ASN
1	U	325	GLU
2	V	60	ASN
1	W	53	ASN
1	W	325	GLU
2	X	60	ASN
3	a	78	LEU
3	a	92	CYS
3	a	178	LEU
3	a	209	LYS
4	b	3	GLN
4	b	11	LEU
4	b	24	GLN
4	b	55	GLN
4	b	90	GLN
4	b	147	GLN
4	b	181	LEU
4	b	188	LYS
3	c	78	LEU
3	c	92	CYS
3	c	113	SER
3	c	178	LEU
3	c	209	LYS
4	d	3	GLN
4	d	11	LEU
4	d	24	GLN
4	d	55	GLN
4	d	90	GLN

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Mol	Chain	Res	Type
4	d	147	GLN
4	d	181	LEU
4	d	188	LYS
3	e	78	LEU
3	e	83	ARG
3	e	92	CYS
3	e	178	LEU
3	e	209	LYS
4	f	3	GLN
4	f	11	LEU
4	f	24	GLN
4	f	55	GLN
4	f	90	GLN
4	f	123	GLU
4	f	147	GLN
4	f	181	LEU
4	f	188	LYS
3	g	78	LEU
3	g	92	CYS
3	g	178	LEU
3	g	209	LYS
4	h	3	GLN
4	h	11	LEU
4	h	24	GLN
4	h	55	GLN
4	h	90	GLN
4	h	123	GLU
4	h	147	GLN
4	h	181	LEU
4	h	188	LYS
3	i	78	LEU
3	i	92	CYS
3	i	113	SER
3	i	115	SER
3	i	178	LEU
3	i	209	LYS
4	j	3	GLN
4	j	11	LEU
4	j	24	GLN
4	j	55	GLN
4	j	90	GLN
4	j	181	LEU

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Mol	Chain	Res	Type
4	j	188	LYS
3	k	78	LEU
3	k	83	ARG
3	k	92	CYS
3	k	178	LEU
3	k	209	LYS
4	l	3	GLN
4	l	11	LEU
4	l	24	GLN
4	l	55	GLN
4	l	90	GLN
4	l	123	GLU
4	l	147	GLN
4	l	181	LEU
4	l	188	LYS
3	m	78	LEU
3	m	92	CYS
3	m	178	LEU
3	m	209	LYS
4	n	3	GLN
4	n	11	LEU
4	n	24	GLN
4	n	55	GLN
4	n	90	GLN
4	n	147	GLN
4	n	181	LEU
4	n	188	LYS
3	o	78	LEU
3	o	83	ARG
3	o	92	CYS
3	o	178	LEU
3	o	209	LYS
4	p	3	GLN
4	p	11	LEU
4	p	24	GLN
4	p	55	GLN
4	p	90	GLN
4	p	123	GLU
4	p	147	GLN
4	p	181	LEU
4	p	188	LYS
3	q	78	LEU

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Mol	Chain	Res	Type
3	q	92	CYS
3	q	178	LEU
3	q	209	LYS
4	r	3	GLN
4	r	11	LEU
4	r	24	GLN
4	r	55	GLN
4	r	90	GLN
4	r	123	GLU
4	r	147	GLN
4	r	181	LEU
4	r	188	LYS
3	s	78	LEU
3	s	92	CYS
3	s	178	LEU
3	s	209	LYS
4	t	3	GLN
4	t	11	LEU
4	t	24	GLN
4	t	55	GLN
4	t	90	GLN
4	t	123	GLU
4	t	147	GLN
4	t	181	LEU
4	t	188	LYS
3	u	78	LEU
3	u	83	ARG
3	u	92	CYS
3	u	178	LEU
3	u	209	LYS
4	v	3	GLN
4	v	11	LEU
4	v	24	GLN
4	v	55	GLN
4	v	90	GLN
4	v	123	GLU
4	v	147	GLN
4	v	181	LEU
4	v	188	LYS
3	w	78	LEU
3	w	92	CYS
3	w	178	LEU

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Mol	Chain	Res	Type
3	w	209	LYS
4	x	3	GLN
4	x	11	LEU
4	x	24	GLN
4	x	55	GLN
4	x	90	GLN
4	x	123	GLU
4	x	147	GLN
4	x	181	LEU
4	x	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	53	ASN
1	A	75	HIS
1	A	137	ASN
1	A	171	ASN
1	A	189	GLN
2	B	12	ASN
2	B	53	ASN
2	B	60	ASN
2	B	159	HIS
1	C	22	ASN
1	C	53	ASN
1	C	75	HIS
1	C	171	ASN
2	D	53	ASN
2	D	60	ASN
2	D	159	HIS
1	E	22	ASN
1	E	53	ASN
1	E	75	HIS
1	E	171	ASN
1	E	189	GLN
2	F	12	ASN
2	F	53	ASN
2	F	60	ASN
2	F	159	HIS
1	G	22	ASN
1	G	53	ASN

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Mol	Chain	Res	Type
1	G	75	HIS
2	H	12	ASN
2	H	53	ASN
2	H	60	ASN
2	H	159	HIS
1	I	22	ASN
1	I	53	ASN
1	I	75	HIS
1	I	171	ASN
1	I	189	GLN
2	J	12	ASN
2	J	53	ASN
2	J	60	ASN
2	J	125	GLN
1	K	22	ASN
1	K	53	ASN
1	K	171	ASN
2	L	12	ASN
2	L	53	ASN
2	L	60	ASN
2	L	65	GLN
2	L	159	HIS
1	M	53	ASN
1	M	75	HIS
1	M	137	ASN
1	M	171	ASN
2	N	12	ASN
2	N	53	ASN
2	N	60	ASN
2	N	159	HIS
1	O	22	ASN
1	O	53	ASN
1	O	75	HIS
1	O	171	ASN
2	P	53	ASN
2	P	60	ASN
2	P	116	ASN
2	P	159	HIS
1	Q	22	ASN
1	Q	53	ASN
1	Q	75	HIS
1	Q	137	ASN

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Mol	Chain	Res	Type
1	Q	171	ASN
2	R	53	ASN
2	R	60	ASN
2	R	159	HIS
1	S	22	ASN
1	S	53	ASN
1	S	75	HIS
1	S	137	ASN
1	S	188	ASN
1	S	189	GLN
2	T	12	ASN
2	T	53	ASN
2	T	60	ASN
2	T	159	HIS
1	U	22	ASN
1	U	53	ASN
1	U	171	ASN
2	V	53	ASN
2	V	60	ASN
2	V	159	HIS
1	W	22	ASN
1	W	53	ASN
1	W	75	HIS
1	W	171	ASN
2	X	53	ASN
2	X	60	ASN
3	a	164	HIS
4	b	55	GLN
4	b	138	ASN
4	b	189	HIS
4	b	199	GLN
3	c	164	HIS
3	c	192	GLN
4	d	55	GLN
4	d	138	ASN
4	d	189	HIS
4	d	199	GLN
3	e	164	HIS
4	f	55	GLN
4	f	137	ASN
4	f	138	ASN
4	f	166	GLN

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Mol	Chain	Res	Type
4	f	189	HIS
4	f	199	GLN
3	g	192	GLN
4	h	55	GLN
4	h	189	HIS
4	h	199	GLN
3	i	39	GLN
3	i	164	HIS
4	j	38	GLN
4	j	55	GLN
4	j	138	ASN
4	j	189	HIS
3	k	164	HIS
4	l	55	GLN
4	l	137	ASN
4	l	138	ASN
4	l	189	HIS
3	m	164	HIS
4	n	55	GLN
4	n	137	ASN
4	n	138	ASN
4	n	189	HIS
4	n	199	GLN
3	o	164	HIS
3	o	192	GLN
4	p	55	GLN
4	p	137	ASN
4	p	138	ASN
4	p	189	HIS
4	p	199	GLN
3	q	164	HIS
3	q	192	GLN
4	r	55	GLN
4	r	137	ASN
4	r	138	ASN
4	r	189	HIS
4	r	199	GLN
3	s	164	HIS
4	t	55	GLN
4	t	137	ASN
4	t	138	ASN
4	t	189	HIS

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Mol	Chain	Res	Type
4	t	199	GLN
3	u	164	HIS
4	v	137	ASN
4	v	138	ASN
4	v	189	HIS
4	v	199	GLN
3	w	39	GLN
3	w	164	HIS
4	x	38	GLN
4	x	55	GLN
4	x	137	ASN
4	x	138	ASN
4	x	189	HIS
4	x	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCA	s	1	3	7,8,9	2.42	2 (28%)	9,10,12	2.33	5 (55%)
3	PCA	w	1	3	7,8,9	2.30	2 (28%)	9,10,12	2.30	5 (55%)
3	PCA	g	1	3	7,8,9	2.20	2 (28%)	9,10,12	2.37	5 (55%)
3	PCA	a	1	3	7,8,9	2.41	2 (28%)	9,10,12	2.32	5 (55%)
3	PCA	i	1	3	7,8,9	2.35	2 (28%)	9,10,12	2.26	5 (55%)
3	PCA	u	1	3	7,8,9	2.31	2 (28%)	9,10,12	2.34	5 (55%)
3	PCA	c	1	3	7,8,9	2.31	2 (28%)	9,10,12	2.35	5 (55%)
3	PCA	o	1	3	7,8,9	2.30	2 (28%)	9,10,12	2.28	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PCA	m	1	3	7,8,9	2.25	2 (28%)	9,10,12	2.15	5 (55%)
3	PCA	k	1	3	7,8,9	2.26	2 (28%)	9,10,12	2.39	5 (55%)
3	PCA	e	1	3	7,8,9	2.29	2 (28%)	9,10,12	2.33	5 (55%)
3	PCA	q	1	3	7,8,9	2.22	2 (28%)	9,10,12	2.27	5 (55%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	s	1	3	-	0/0/11/13	0/1/1/1
3	PCA	w	1	3	-	0/0/11/13	0/1/1/1
3	PCA	g	1	3	-	0/0/11/13	0/1/1/1
3	PCA	a	1	3	-	0/0/11/13	0/1/1/1
3	PCA	i	1	3	-	0/0/11/13	0/1/1/1
3	PCA	u	1	3	-	0/0/11/13	0/1/1/1
3	PCA	c	1	3	-	0/0/11/13	0/1/1/1
3	PCA	o	1	3	-	0/0/11/13	0/1/1/1
3	PCA	m	1	3	-	0/0/11/13	0/1/1/1
3	PCA	k	1	3	-	0/0/11/13	0/1/1/1
3	PCA	e	1	3	-	0/0/11/13	0/1/1/1
3	PCA	q	1	3	-	0/0/11/13	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1	PCA	CD-N	5.13	1.47	1.34
3	s	1	PCA	CD-N	5.11	1.47	1.34
3	i	1	PCA	CD-N	5.09	1.47	1.34
3	c	1	PCA	CD-N	5.07	1.47	1.34
3	u	1	PCA	CD-N	5.05	1.47	1.34
3	k	1	PCA	CD-N	5.00	1.46	1.34
3	e	1	PCA	CD-N	4.98	1.46	1.34
3	o	1	PCA	CD-N	4.98	1.46	1.34
3	w	1	PCA	CD-N	4.95	1.46	1.34
3	g	1	PCA	CD-N	4.93	1.46	1.34
3	m	1	PCA	CD-N	4.91	1.46	1.34
3	q	1	PCA	CD-N	4.89	1.46	1.34
3	s	1	PCA	CA-N	3.68	1.50	1.46
3	a	1	PCA	CA-N	3.61	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	i	1	PCA	CA-N	3.38	1.50	1.46
3	w	1	PCA	CA-N	3.34	1.50	1.46
3	o	1	PCA	CA-N	3.32	1.50	1.46
3	e	1	PCA	CA-N	3.29	1.50	1.46
3	c	1	PCA	CA-N	3.24	1.50	1.46
3	u	1	PCA	CA-N	3.24	1.50	1.46
3	m	1	PCA	CA-N	3.19	1.50	1.46
3	k	1	PCA	CA-N	3.06	1.50	1.46
3	q	1	PCA	CA-N	3.04	1.50	1.46
3	g	1	PCA	CA-N	2.87	1.49	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	1	PCA	CB-CA-C	-3.89	107.32	112.66
3	s	1	PCA	CB-CA-C	-3.89	107.32	112.66
3	o	1	PCA	CB-CA-C	-3.57	107.76	112.66
3	a	1	PCA	CB-CA-C	-3.56	107.77	112.66
3	w	1	PCA	CB-CA-C	-3.53	107.81	112.66
3	g	1	PCA	CB-CA-C	-3.42	107.97	112.66
3	c	1	PCA	CB-CA-C	-3.39	108.01	112.66
3	q	1	PCA	CB-CA-C	-3.33	108.09	112.66
3	u	1	PCA	CB-CA-C	-3.32	108.11	112.66
3	k	1	PCA	OE-CD-CG	-3.32	120.80	126.72
3	u	1	PCA	OE-CD-CG	-3.27	120.89	126.72
3	k	1	PCA	CA-N-CD	-3.24	102.48	113.58
3	c	1	PCA	OE-CD-CG	-3.21	120.98	126.72
3	i	1	PCA	CA-N-CD	-3.19	102.66	113.58
3	a	1	PCA	OE-CD-CG	-3.18	121.04	126.72
3	g	1	PCA	CA-N-CD	-3.16	102.77	113.58
3	c	1	PCA	CA-N-CD	-3.12	102.90	113.58
3	i	1	PCA	CB-CA-N	3.11	111.79	103.24
3	k	1	PCA	CB-CA-N	3.09	111.75	103.24
3	s	1	PCA	OE-CD-CG	-3.08	121.23	126.72
3	g	1	PCA	OE-CD-CG	-3.07	121.24	126.72
3	u	1	PCA	CA-N-CD	-3.07	103.06	113.58
3	m	1	PCA	CB-CA-C	-3.06	108.46	112.66
3	w	1	PCA	CA-N-CD	-3.03	103.21	113.58
3	q	1	PCA	CA-N-CD	-3.01	103.26	113.58
3	i	1	PCA	OE-CD-CG	-3.00	121.36	126.72
3	g	1	PCA	CB-CA-N	2.99	111.47	103.24
3	c	1	PCA	CB-CA-N	2.96	111.38	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	1	PCA	CA-N-CD	-2.96	103.45	113.58
3	o	1	PCA	CA-N-CD	-2.96	103.45	113.58
3	k	1	PCA	CB-CA-C	-2.95	108.61	112.66
3	a	1	PCA	CA-N-CD	-2.93	103.53	113.58
3	m	1	PCA	CA-N-CD	-2.93	103.53	113.58
3	w	1	PCA	OE-CD-CG	-2.90	121.54	126.72
3	s	1	PCA	CA-N-CD	-2.90	103.67	113.58
3	m	1	PCA	CB-CA-N	2.89	111.18	103.24
3	o	1	PCA	OE-CD-CG	-2.89	121.57	126.72
3	q	1	PCA	CB-CA-N	2.88	111.17	103.24
3	u	1	PCA	CB-CA-N	2.87	111.12	103.24
3	w	1	PCA	CB-CA-N	2.86	111.11	103.24
3	e	1	PCA	OE-CD-CG	-2.85	121.64	126.72
3	i	1	PCA	CB-CA-C	-2.81	108.80	112.66
3	q	1	PCA	OE-CD-CG	-2.81	121.71	126.72
3	e	1	PCA	CB-CA-N	2.81	110.97	103.24
3	k	1	PCA	CG-CD-N	2.80	115.25	108.39
3	g	1	PCA	CG-CD-N	2.79	115.22	108.39
3	o	1	PCA	CB-CA-N	2.77	110.86	103.24
3	u	1	PCA	CG-CD-N	2.69	114.97	108.39
3	a	1	PCA	CB-CA-N	2.68	110.62	103.24
3	c	1	PCA	CG-CD-N	2.66	114.89	108.39
3	i	1	PCA	CG-CD-N	2.65	114.86	108.39
3	s	1	PCA	CB-CA-N	2.61	110.41	103.24
3	w	1	PCA	CG-CD-N	2.60	114.76	108.39
3	q	1	PCA	CG-CD-N	2.59	114.73	108.39
3	o	1	PCA	CG-CD-N	2.56	114.65	108.39
3	a	1	PCA	CG-CD-N	2.55	114.63	108.39
3	s	1	PCA	CG-CD-N	2.55	114.62	108.39
3	e	1	PCA	CG-CD-N	2.51	114.54	108.39
3	m	1	PCA	OE-CD-CG	-2.47	122.30	126.72
3	m	1	PCA	CG-CD-N	2.46	114.42	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

72 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	0	1	5,1	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
5	NAG	0	2	5	14,14,15	0.58	0	17,19,21	0.74	0
5	BMA	0	3	5	11,11,12	0.73	0	15,15,17	0.89	1 (6%)
5	MAN	0	4	5	11,11,12	0.66	0	15,15,17	0.67	0
6	NAG	1	1	6,1	14,14,15	0.59	0	17,19,21	0.64	0
6	NAG	1	2	6	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
5	NAG	2	1	5,1	14,14,15	0.61	0	17,19,21	0.98	0
5	NAG	2	2	5	14,14,15	0.54	0	17,19,21	0.78	0
5	BMA	2	3	5	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
5	MAN	2	4	5	11,11,12	0.58	0	15,15,17	0.65	0
6	NAG	3	1	6,1	14,14,15	0.52	0	17,19,21	0.79	0
6	NAG	3	2	6	14,14,15	0.47	0	17,19,21	1.06	1 (5%)
5	NAG	4	1	5,1	14,14,15	0.50	0	17,19,21	0.87	0
5	NAG	4	2	5	14,14,15	0.54	0	17,19,21	0.69	0
5	BMA	4	3	5	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
5	MAN	4	4	5	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	5	1	6,1	14,14,15	0.58	0	17,19,21	0.60	0
6	NAG	5	2	6	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
5	NAG	6	1	5,1	14,14,15	0.49	0	17,19,21	0.92	1 (5%)
5	NAG	6	2	5	14,14,15	0.53	0	17,19,21	0.70	0
5	BMA	6	3	5	11,11,12	0.75	0	15,15,17	0.92	1 (6%)
5	MAN	6	4	5	11,11,12	0.60	0	15,15,17	0.54	0
6	NAG	7	1	6,1	14,14,15	0.56	0	17,19,21	0.57	0
6	NAG	7	2	6	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
5	NAG	8	1	5,1	14,14,15	0.45	0	17,19,21	1.20	1 (5%)
5	NAG	8	2	5	14,14,15	0.52	0	17,19,21	0.76	0
5	BMA	8	3	5	11,11,12	0.68	0	15,15,17	0.89	1 (6%)
5	MAN	8	4	5	11,11,12	0.62	0	15,15,17	0.81	0
6	NAG	9	1	6,1	14,14,15	0.58	0	17,19,21	0.66	0
6	NAG	9	2	6	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
5	NAG	AA	1	5,1	14,14,15	0.58	0	17,19,21	0.91	1 (5%)
5	NAG	AA	2	5	14,14,15	0.57	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	AA	3	5	11,11,12	0.82	0	15,15,17	0.91	1 (6%)
5	MAN	AA	4	5	11,11,12	0.61	0	15,15,17	0.78	0
6	NAG	BA	1	6,1	14,14,15	0.55	0	17,19,21	0.64	0
6	NAG	BA	2	6	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
5	NAG	CA	1	5,1	14,14,15	0.50	0	17,19,21	0.90	0
5	NAG	CA	2	5	14,14,15	0.54	0	17,19,21	0.90	0
5	BMA	CA	3	5	11,11,12	0.78	0	15,15,17	0.93	1 (6%)
5	MAN	CA	4	5	11,11,12	0.61	0	15,15,17	0.64	0
6	NAG	DA	1	6,1	14,14,15	0.60	0	17,19,21	0.78	0
6	NAG	DA	2	6	14,14,15	0.52	0	17,19,21	0.83	1 (5%)
5	NAG	EA	1	5,1	14,14,15	0.46	0	17,19,21	0.98	1 (5%)
5	NAG	EA	2	5	14,14,15	0.54	0	17,19,21	0.96	1 (5%)
5	BMA	EA	3	5	11,11,12	0.75	0	15,15,17	0.96	1 (6%)
5	MAN	EA	4	5	11,11,12	0.61	0	15,15,17	0.59	0
6	NAG	FA	1	6,1	14,14,15	0.58	0	17,19,21	0.67	0
6	NAG	FA	2	6	14,14,15	0.55	0	17,19,21	0.77	1 (5%)
5	NAG	GA	1	5,1	14,14,15	0.54	0	17,19,21	1.10	0
5	NAG	GA	2	5	14,14,15	0.55	0	17,19,21	0.94	0
5	BMA	GA	3	5	11,11,12	0.77	0	15,15,17	0.86	1 (6%)
5	MAN	GA	4	5	11,11,12	0.60	0	15,15,17	0.60	0
6	NAG	HA	1	6,1	14,14,15	0.53	0	17,19,21	0.69	0
6	NAG	HA	2	6	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
5	NAG	IA	1	5,1	14,14,15	0.48	0	17,19,21	0.94	0
5	NAG	IA	2	5	14,14,15	0.56	0	17,19,21	0.62	0
5	BMA	IA	3	5	11,11,12	0.74	0	15,15,17	0.86	1 (6%)
5	MAN	IA	4	5	11,11,12	0.58	0	15,15,17	0.64	0
6	NAG	JA	1	6,1	14,14,15	0.58	0	17,19,21	0.57	0
6	NAG	JA	2	6	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
5	NAG	Y	1	5,1	14,14,15	0.48	0	17,19,21	1.12	1 (5%)
5	NAG	Y	2	5	14,14,15	0.66	0	17,19,21	1.08	2 (11%)
5	BMA	Y	3	5	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
5	MAN	Y	4	5	11,11,12	0.60	0	15,15,17	0.56	0
6	NAG	Z	1	6,1	14,14,15	0.55	0	17,19,21	0.49	0
6	NAG	Z	2	6	14,14,15	0.47	0	17,19,21	0.68	0
5	NAG	y	1	5,1	14,14,15	0.52	0	17,19,21	0.85	0
5	NAG	y	2	5	14,14,15	0.54	0	17,19,21	0.61	0
5	BMA	y	3	5	11,11,12	0.70	0	15,15,17	1.15	2 (13%)
5	MAN	y	4	5	11,11,12	0.61	0	15,15,17	0.58	0
6	NAG	z	1	6,1	14,14,15	0.61	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	z	2	6	14,14,15	0.44	0	17,19,21	0.90	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	0	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	BMA	0	3	5	-	0/2/19/22	0/1/1/1
5	MAN	0	4	5	-	1/2/19/22	0/1/1/1
6	NAG	1	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	1	2	6	-	0/6/23/26	0/1/1/1
5	NAG	2	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	2	2	5	-	0/6/23/26	0/1/1/1
5	BMA	2	3	5	-	0/2/19/22	0/1/1/1
5	MAN	2	4	5	-	2/2/19/22	0/1/1/1
6	NAG	3	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	3	2	6	-	0/6/23/26	0/1/1/1
5	NAG	4	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	4	2	5	-	0/6/23/26	0/1/1/1
5	BMA	4	3	5	-	0/2/19/22	0/1/1/1
5	MAN	4	4	5	-	0/2/19/22	0/1/1/1
6	NAG	5	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	5	2	6	-	0/6/23/26	0/1/1/1
5	NAG	6	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	6	2	5	-	0/6/23/26	0/1/1/1
5	BMA	6	3	5	-	0/2/19/22	0/1/1/1
5	MAN	6	4	5	-	0/2/19/22	0/1/1/1
6	NAG	7	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	7	2	6	-	0/6/23/26	0/1/1/1
5	NAG	8	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	8	2	5	-	0/6/23/26	0/1/1/1
5	BMA	8	3	5	-	0/2/19/22	0/1/1/1
5	MAN	8	4	5	-	2/2/19/22	0/1/1/1
6	NAG	9	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	9	2	6	-	0/6/23/26	0/1/1/1
5	NAG	AA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	AA	3	5	-	1/2/19/22	0/1/1/1
5	MAN	AA	4	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	BA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	BA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	CA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	CA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	CA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	CA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	DA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	EA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	EA	2	5	-	2/6/23/26	0/1/1/1
5	BMA	EA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	EA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	FA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	FA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	GA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	GA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	GA	3	5	-	1/2/19/22	0/1/1/1
5	MAN	GA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	HA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	HA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	IA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	IA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	IA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	IA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	JA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	JA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
5	NAG	y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	y	4	5	-	0/2/19/22	0/1/1/1
6	NAG	z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	z	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3	2	NAG	C1-O5-C5	3.34	116.67	112.19
5	8	1	NAG	C1-O5-C5	3.26	116.55	112.19
5	Y	3	BMA	C1-C2-C3	3.12	114.19	109.64
5	2	3	BMA	C1-C2-C3	2.98	113.99	109.64
6	1	2	NAG	C1-O5-C5	2.96	116.16	112.19
6	z	2	NAG	C1-O5-C5	2.85	116.01	112.19
6	7	2	NAG	C1-O5-C5	2.83	115.98	112.19
5	EA	3	BMA	C1-C2-C3	2.81	113.73	109.64
5	Y	1	NAG	O5-C1-C2	-2.74	107.05	111.29
6	9	2	NAG	C1-O5-C5	2.67	115.76	112.19
6	JA	2	NAG	C1-O5-C5	2.64	115.73	112.19
5	4	3	BMA	C1-C2-C3	2.62	113.46	109.64
5	y	3	BMA	C1-C2-C3	2.59	113.42	109.64
5	IA	3	BMA	C1-C2-C3	2.56	113.37	109.64
5	CA	3	BMA	C1-C2-C3	2.55	113.36	109.64
5	6	1	NAG	O5-C1-C2	-2.52	107.39	111.29
6	HA	2	NAG	C1-O5-C5	2.50	115.53	112.19
5	Y	2	NAG	O5-C5-C6	2.45	112.43	107.66
6	5	2	NAG	C1-O5-C5	2.45	115.46	112.19
6	DA	2	NAG	C1-O5-C5	2.44	115.46	112.19
5	GA	3	BMA	C1-C2-C3	2.44	113.19	109.64
5	AA	3	BMA	C1-C2-C3	2.43	113.18	109.64
5	6	3	BMA	C1-C2-C3	2.42	113.17	109.64
5	0	3	BMA	C1-C2-C3	2.41	113.15	109.64
5	8	3	BMA	C1-C2-C3	2.39	113.13	109.64
5	y	3	BMA	O5-C5-C4	-2.26	105.34	110.83
6	BA	2	NAG	C1-O5-C5	2.18	115.11	112.19
5	AA	1	NAG	O5-C1-C2	-2.17	107.93	111.29
5	Y	2	NAG	C1-O5-C5	-2.16	109.29	112.19
5	Y	3	BMA	C1-O5-C5	2.16	115.08	112.19
5	EA	1	NAG	C1-O5-C5	2.14	115.05	112.19
5	0	1	NAG	O5-C1-C2	-2.05	108.11	111.29
5	EA	2	NAG	O6-C6-C5	2.00	118.16	111.33
6	FA	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	8	4	MAN	C4-C5-C6-O6
5	EA	2	NAG	C4-C5-C6-O6
5	EA	2	NAG	O5-C5-C6-O6
5	AA	4	MAN	C4-C5-C6-O6

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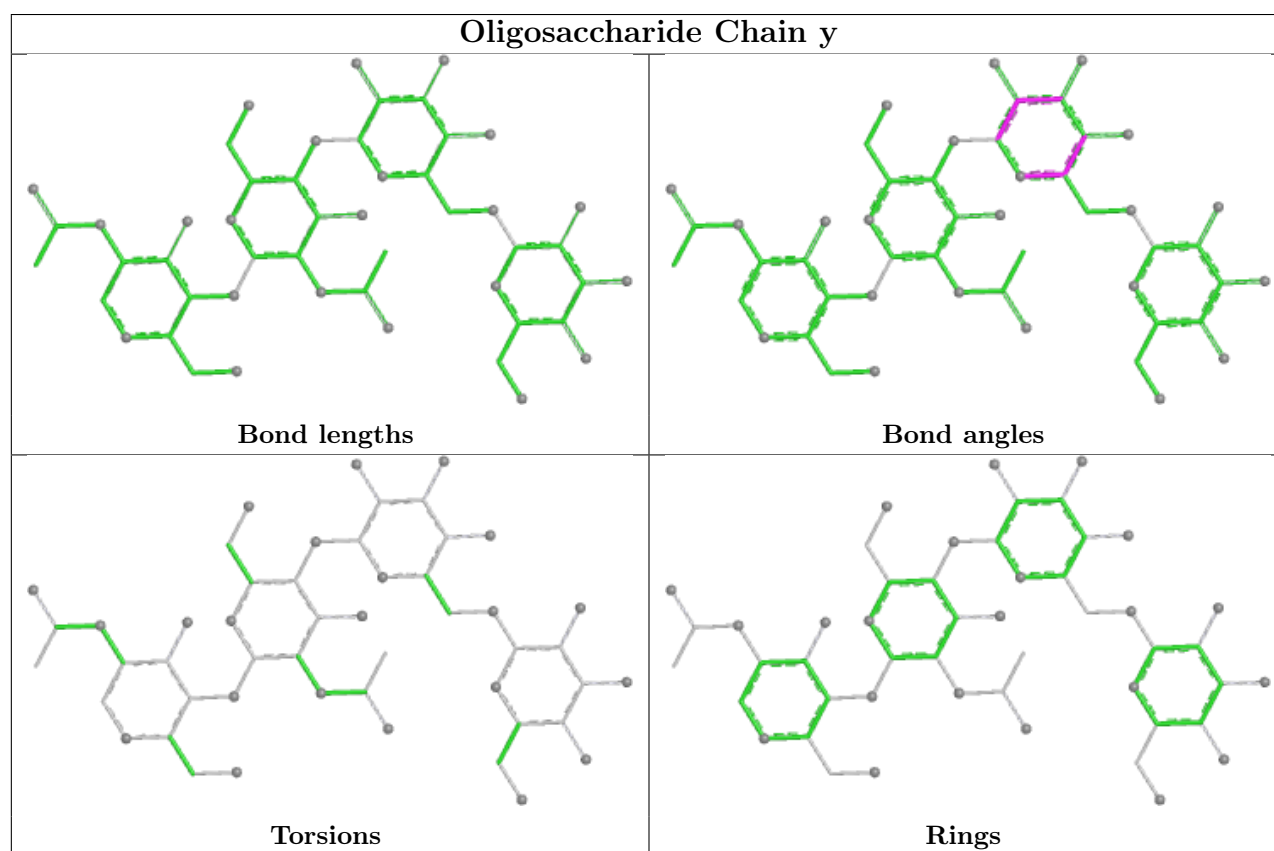
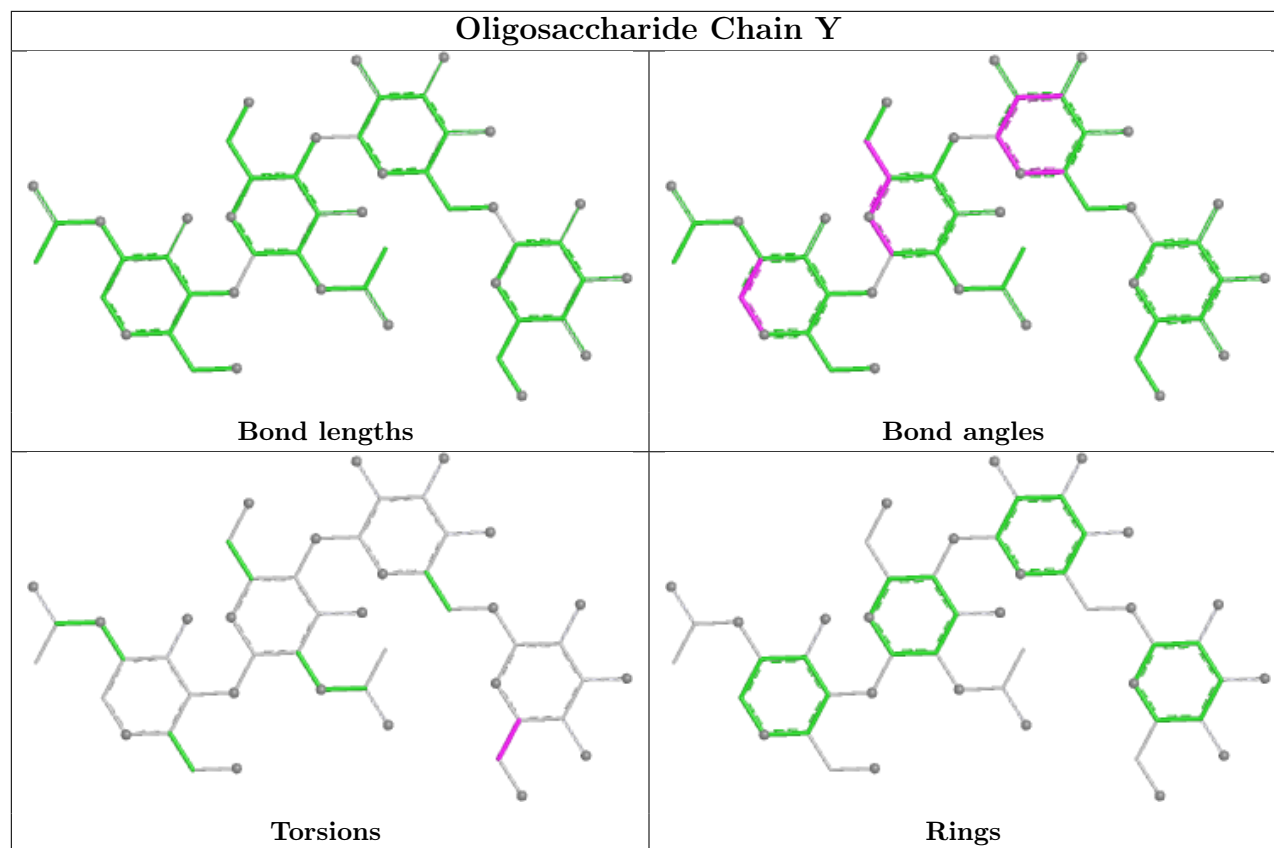
Mol	Chain	Res	Type	Atoms
5	CA	4	MAN	C4-C5-C6-O6
5	8	4	MAN	O5-C5-C6-O6
5	Y	4	MAN	C4-C5-C6-O6
5	CA	4	MAN	O5-C5-C6-O6
5	2	4	MAN	C4-C5-C6-O6
5	GA	4	MAN	C4-C5-C6-O6
5	EA	4	MAN	C4-C5-C6-O6
5	IA	4	MAN	C4-C5-C6-O6
5	AA	4	MAN	O5-C5-C6-O6
5	Y	4	MAN	O5-C5-C6-O6
5	0	4	MAN	C4-C5-C6-O6
5	GA	4	MAN	O5-C5-C6-O6
5	GA	3	BMA	O5-C5-C6-O6
5	EA	4	MAN	O5-C5-C6-O6
5	2	4	MAN	O5-C5-C6-O6
5	IA	4	MAN	O5-C5-C6-O6
5	AA	3	BMA	O5-C5-C6-O6

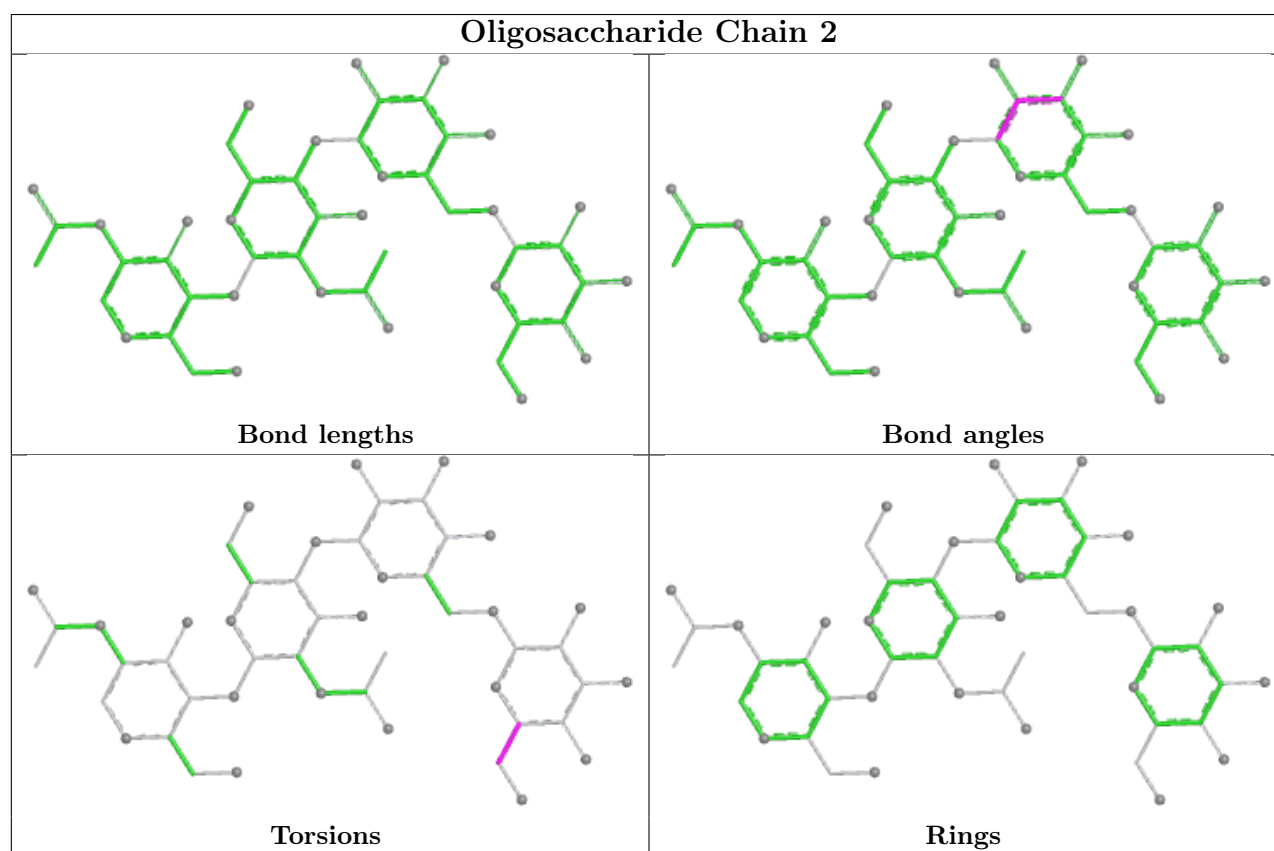
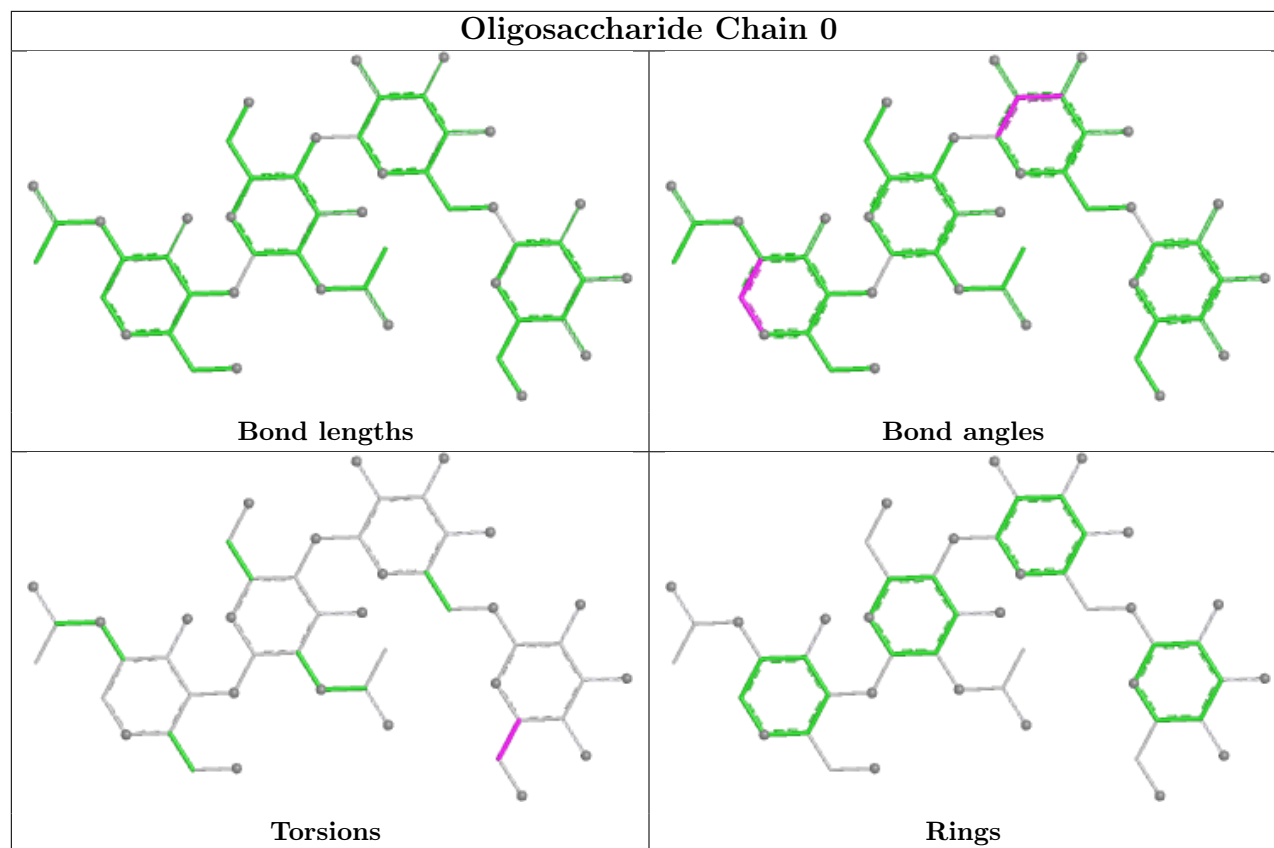
There are no ring outliers.

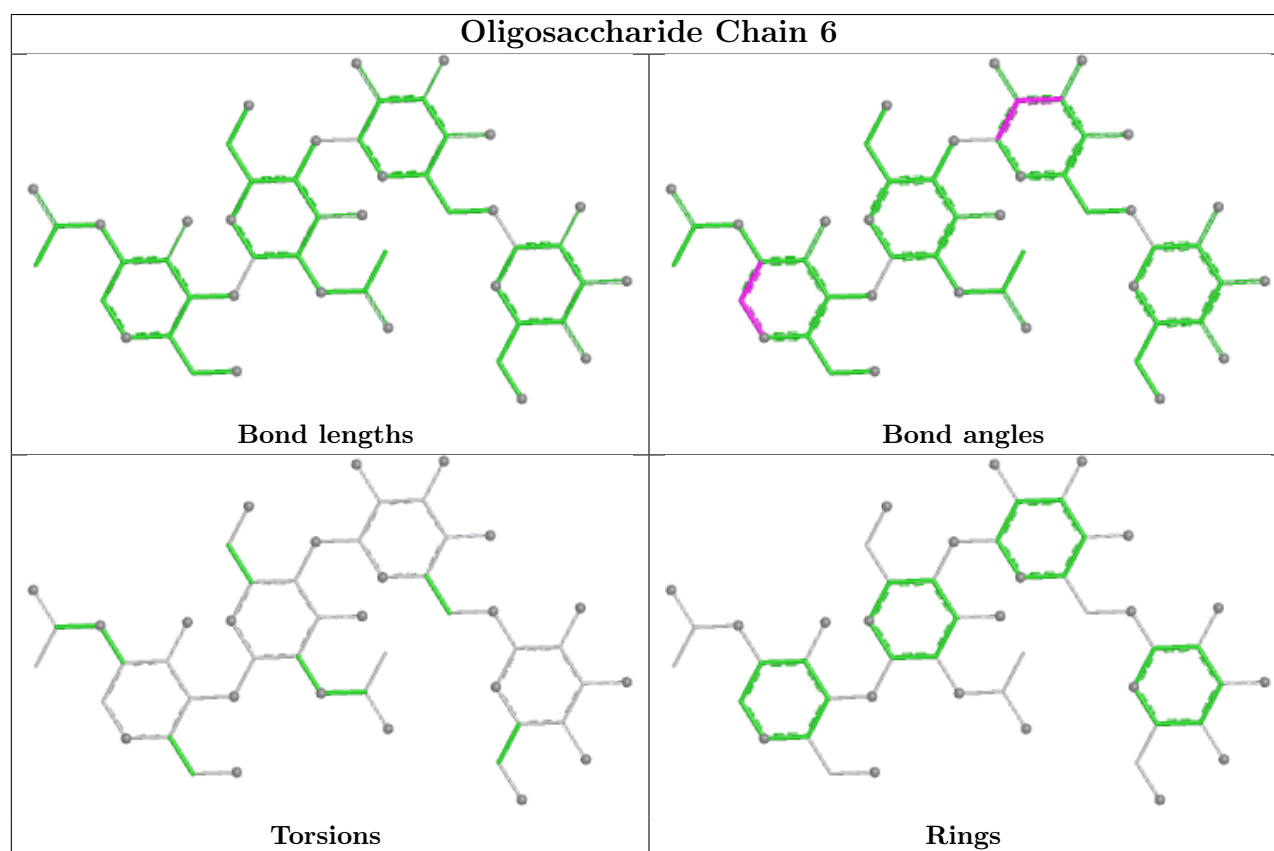
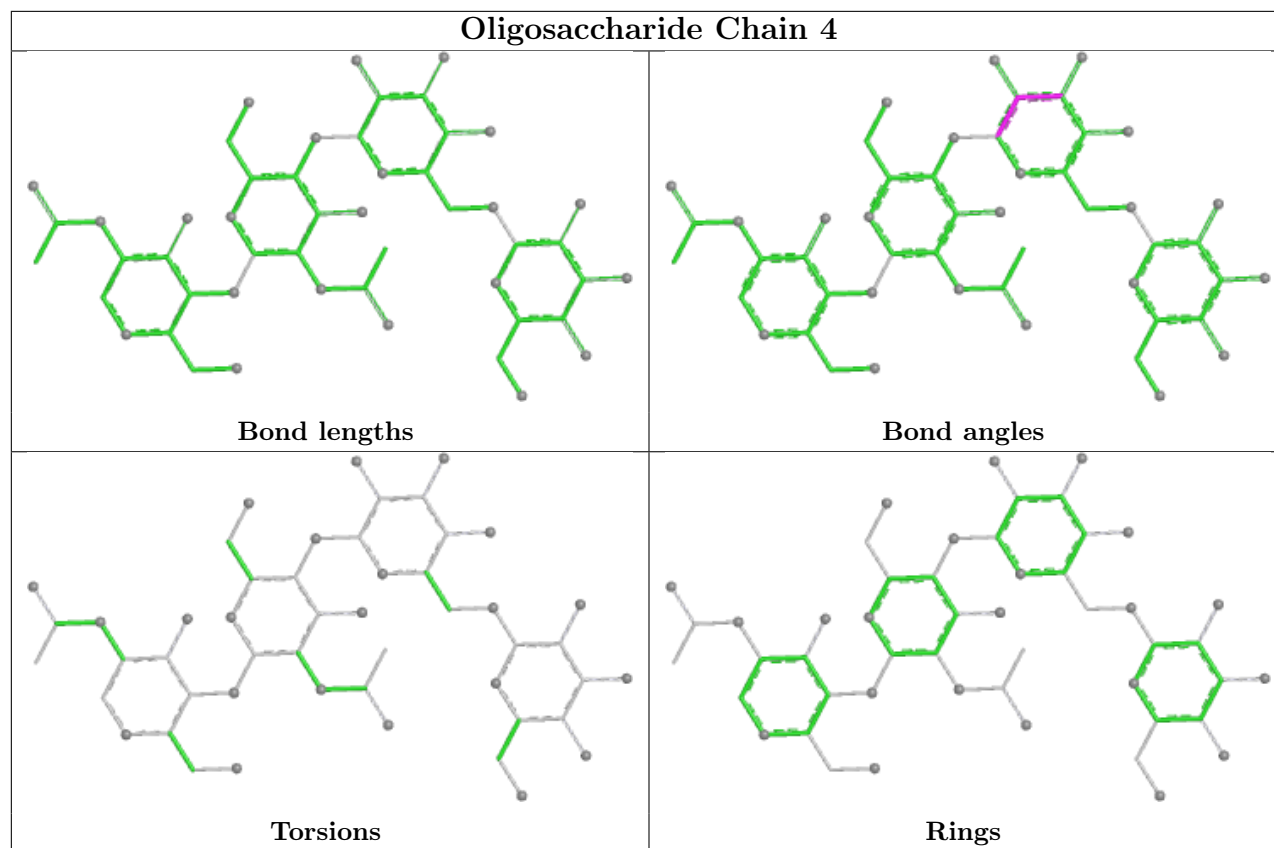
1 monomer is involved in 1 short contact:

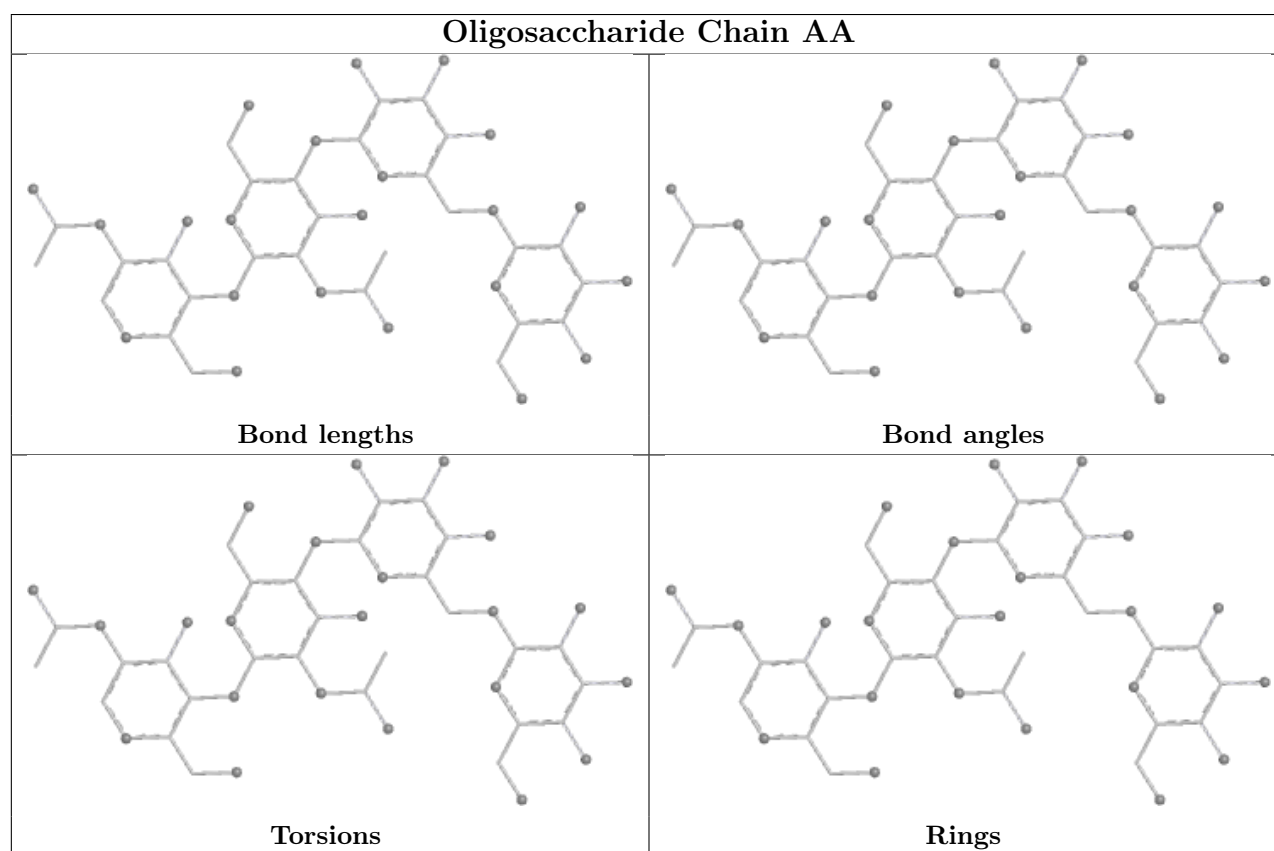
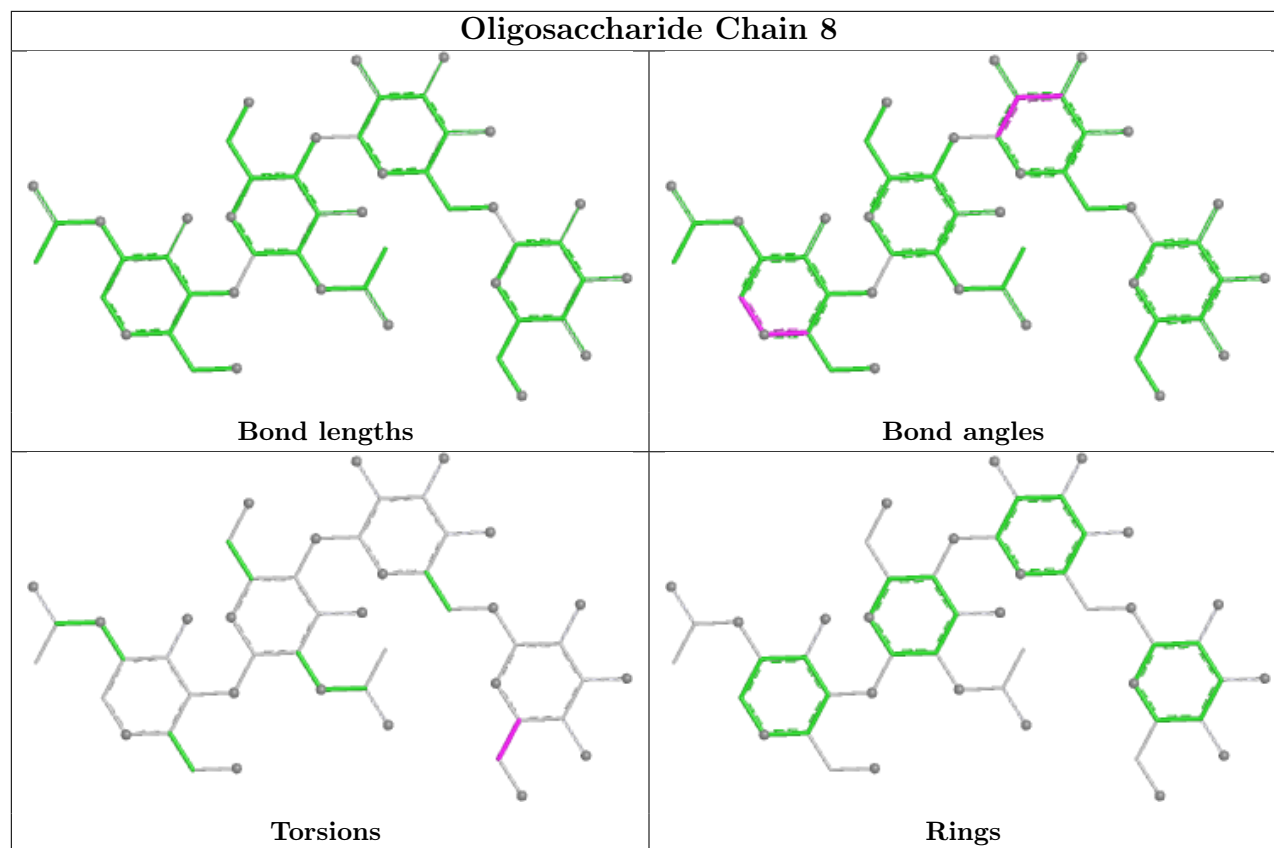
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	EA	1	NAG	1	0

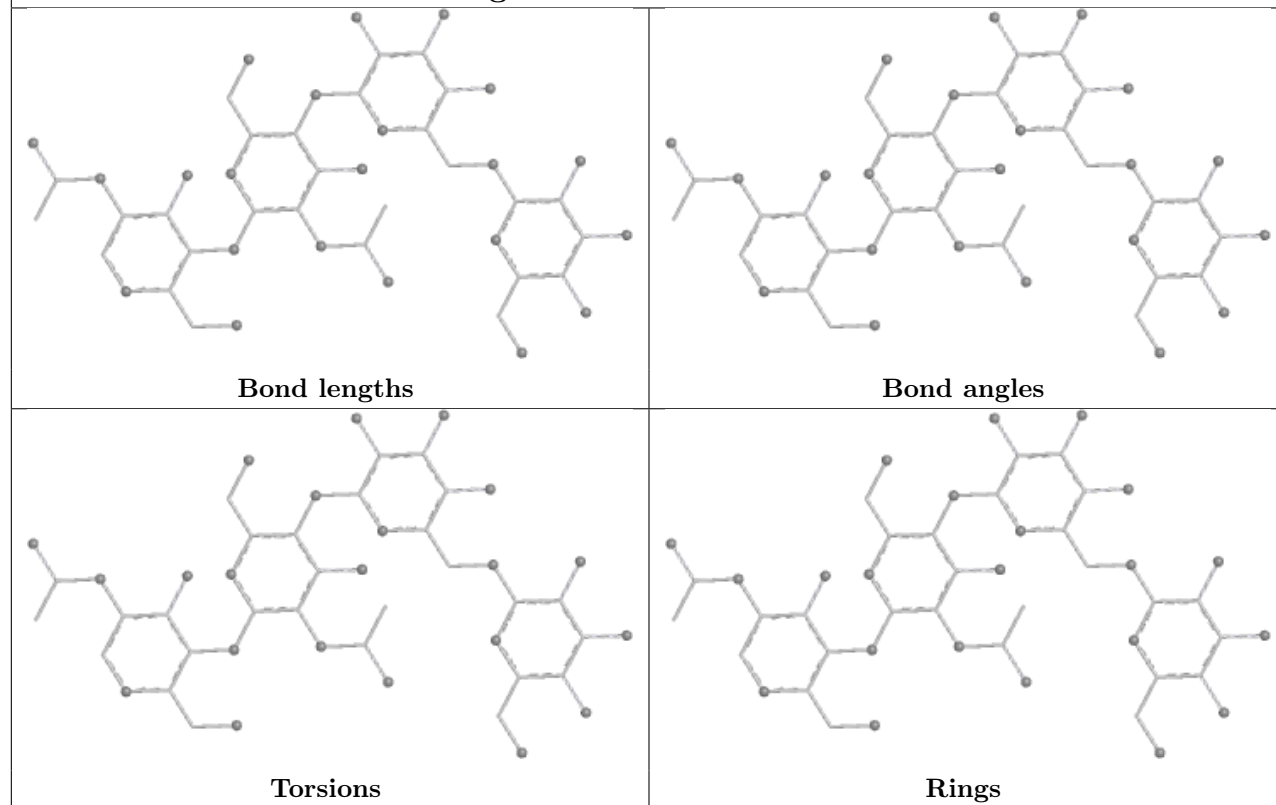
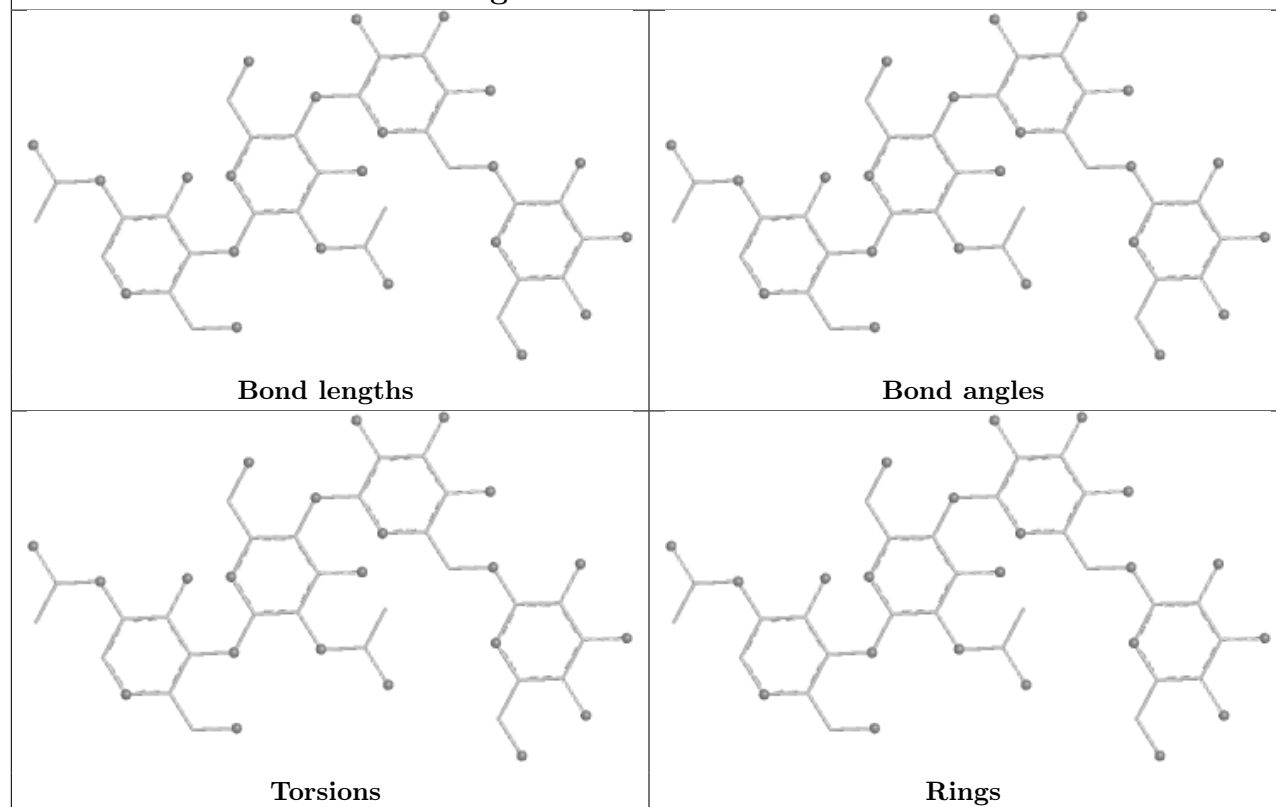
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

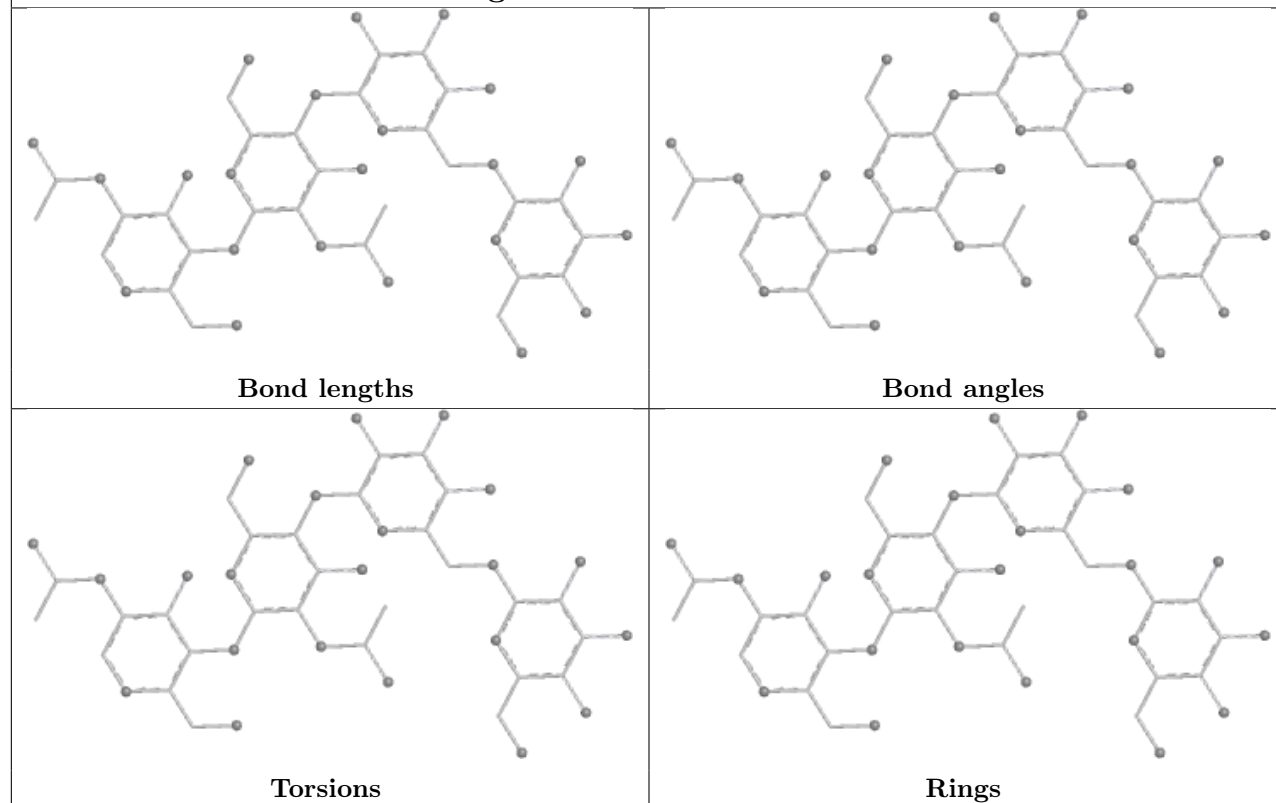
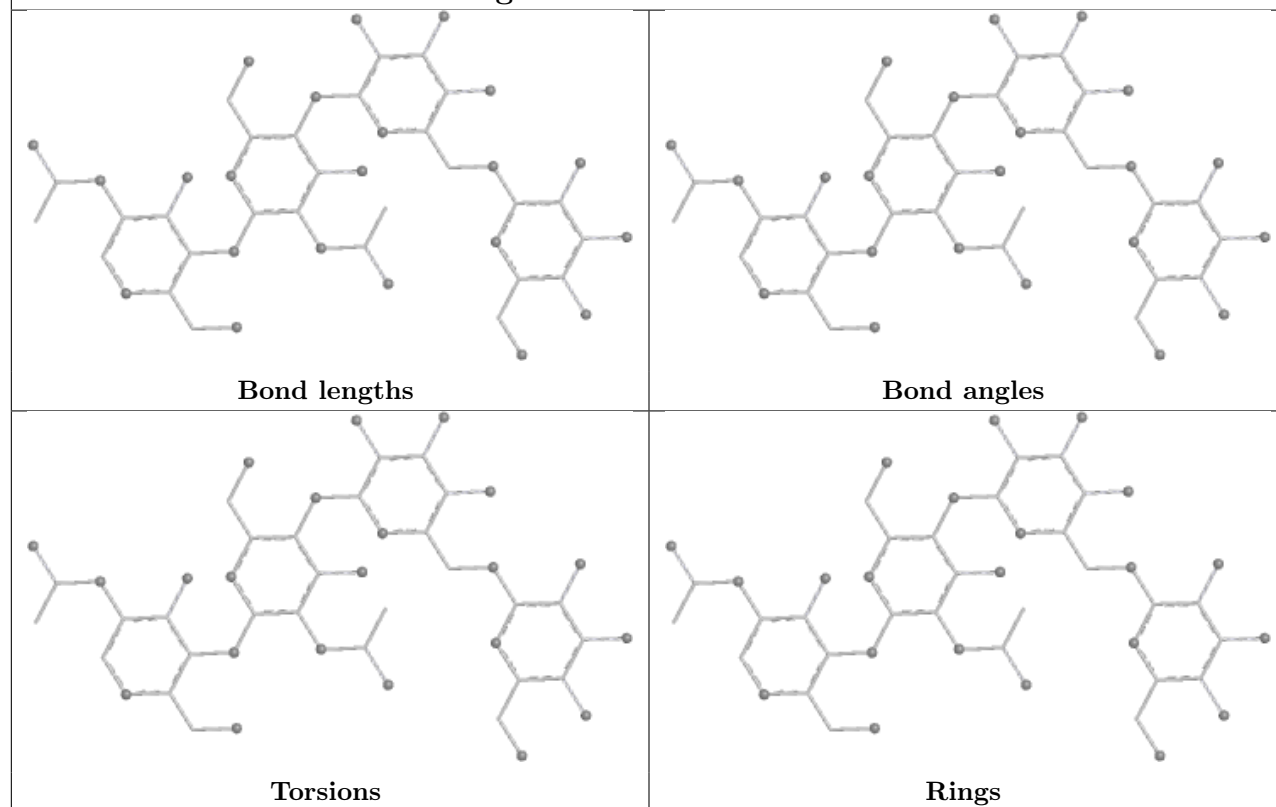


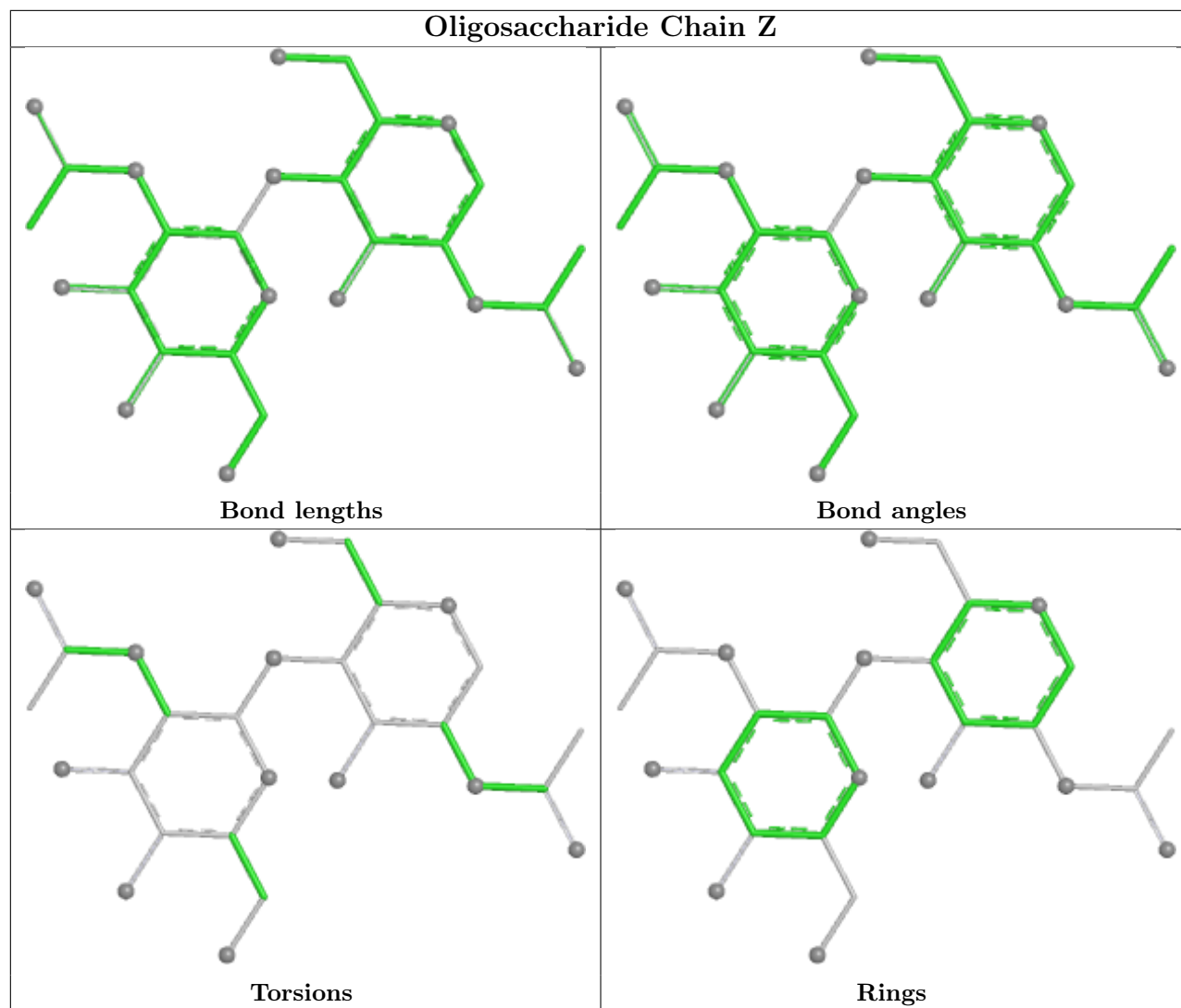


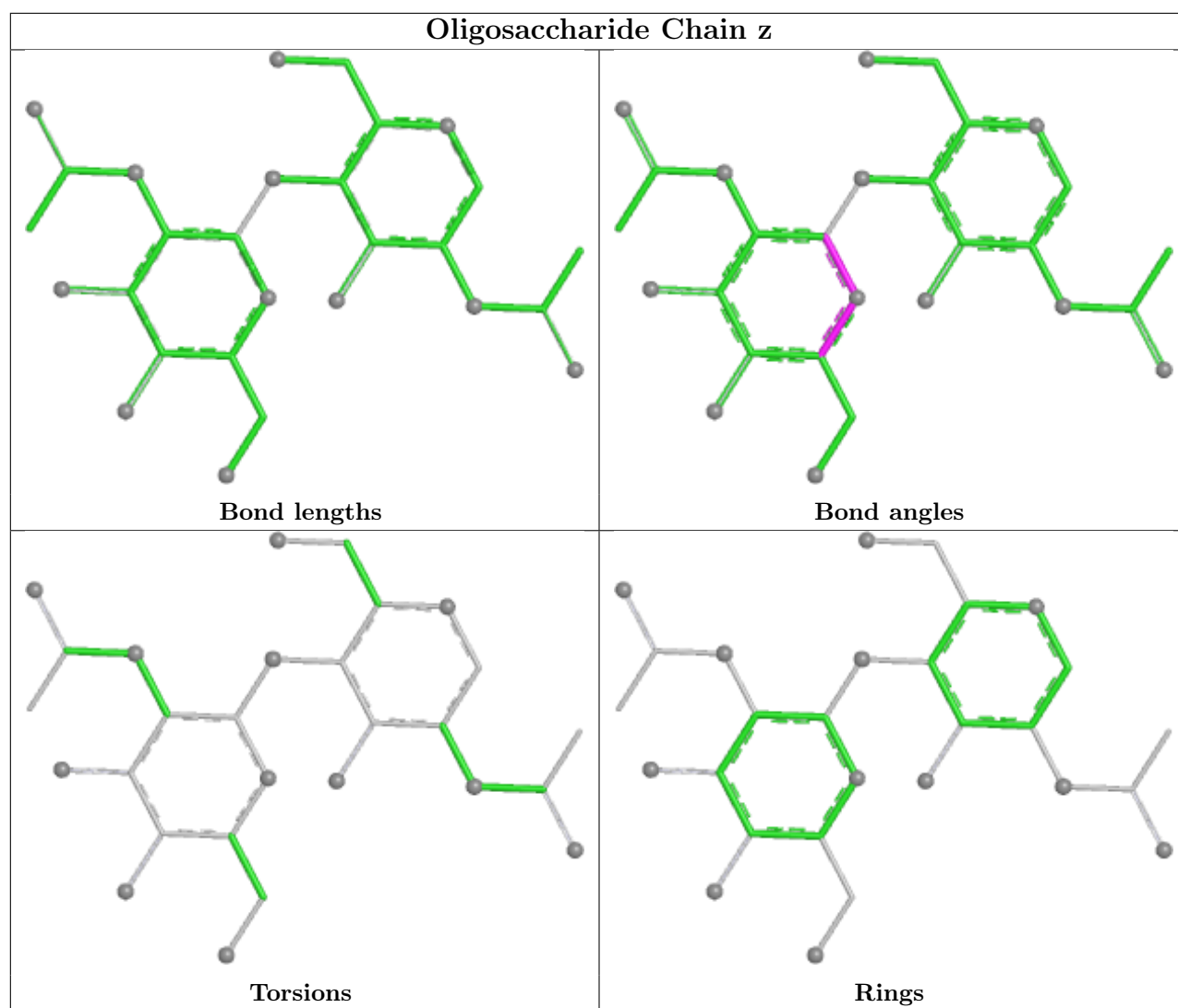


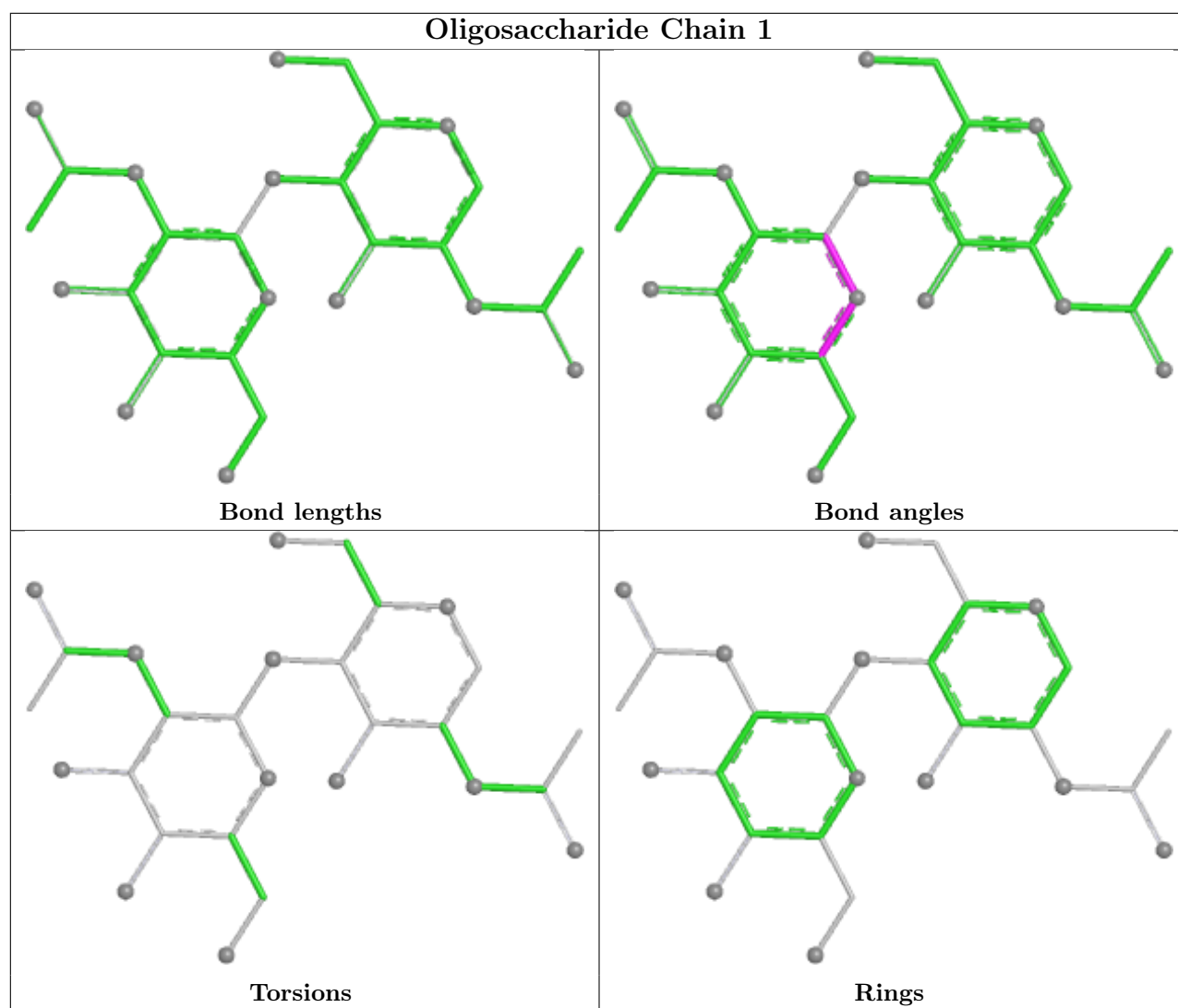


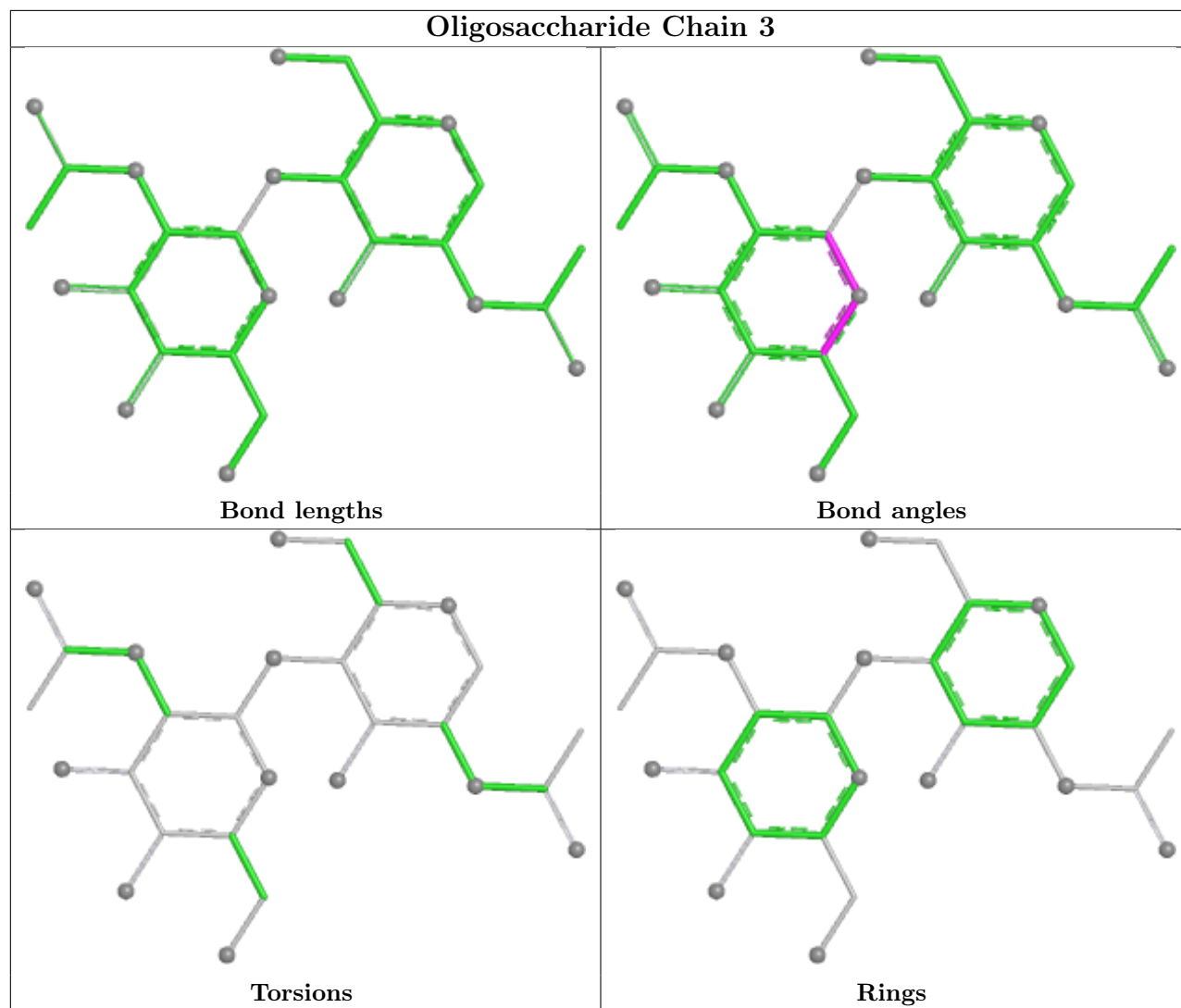
Oligosaccharide Chain CA**Oligosaccharide Chain EA**

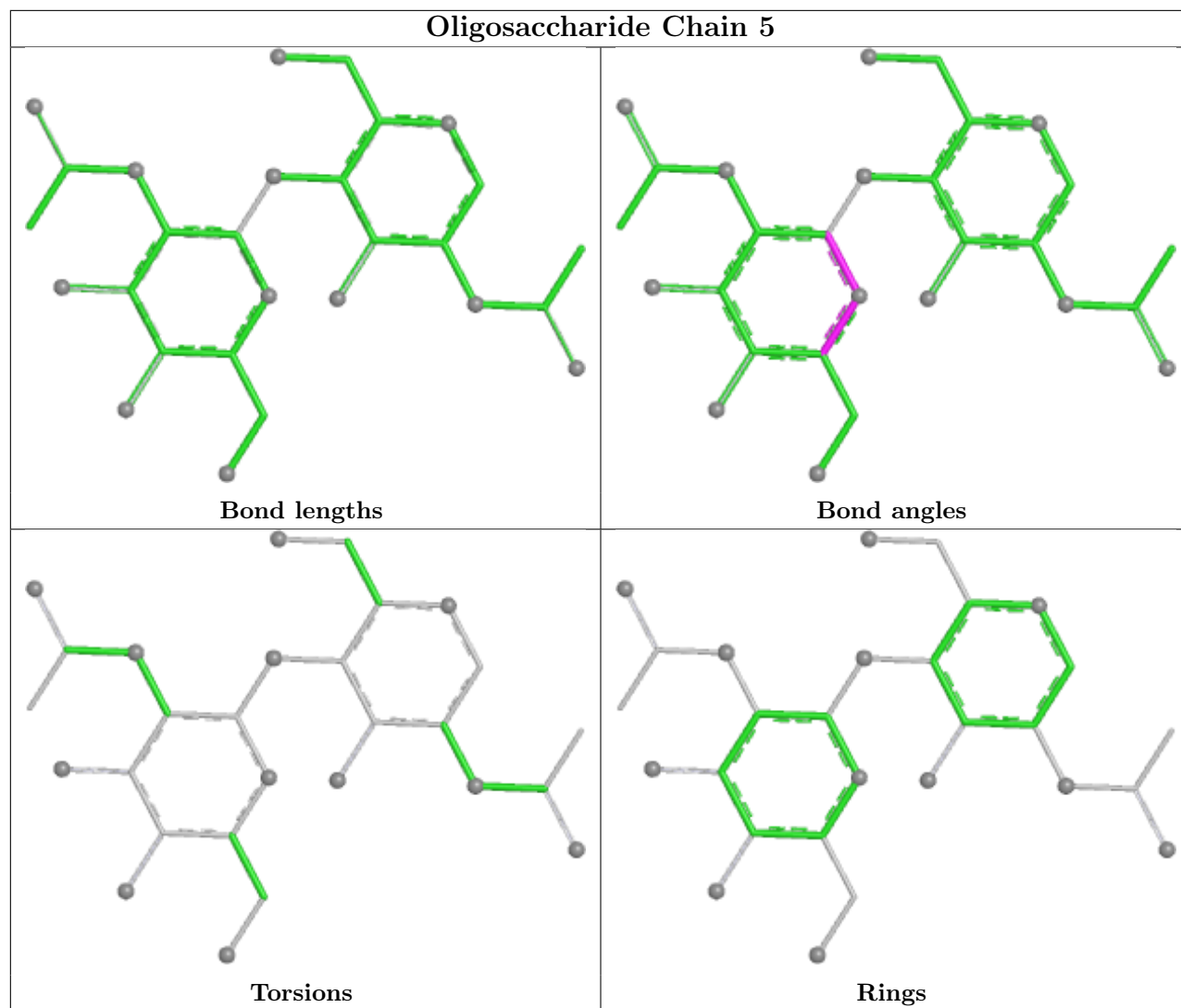
Oligosaccharide Chain GA**Oligosaccharide Chain IA**

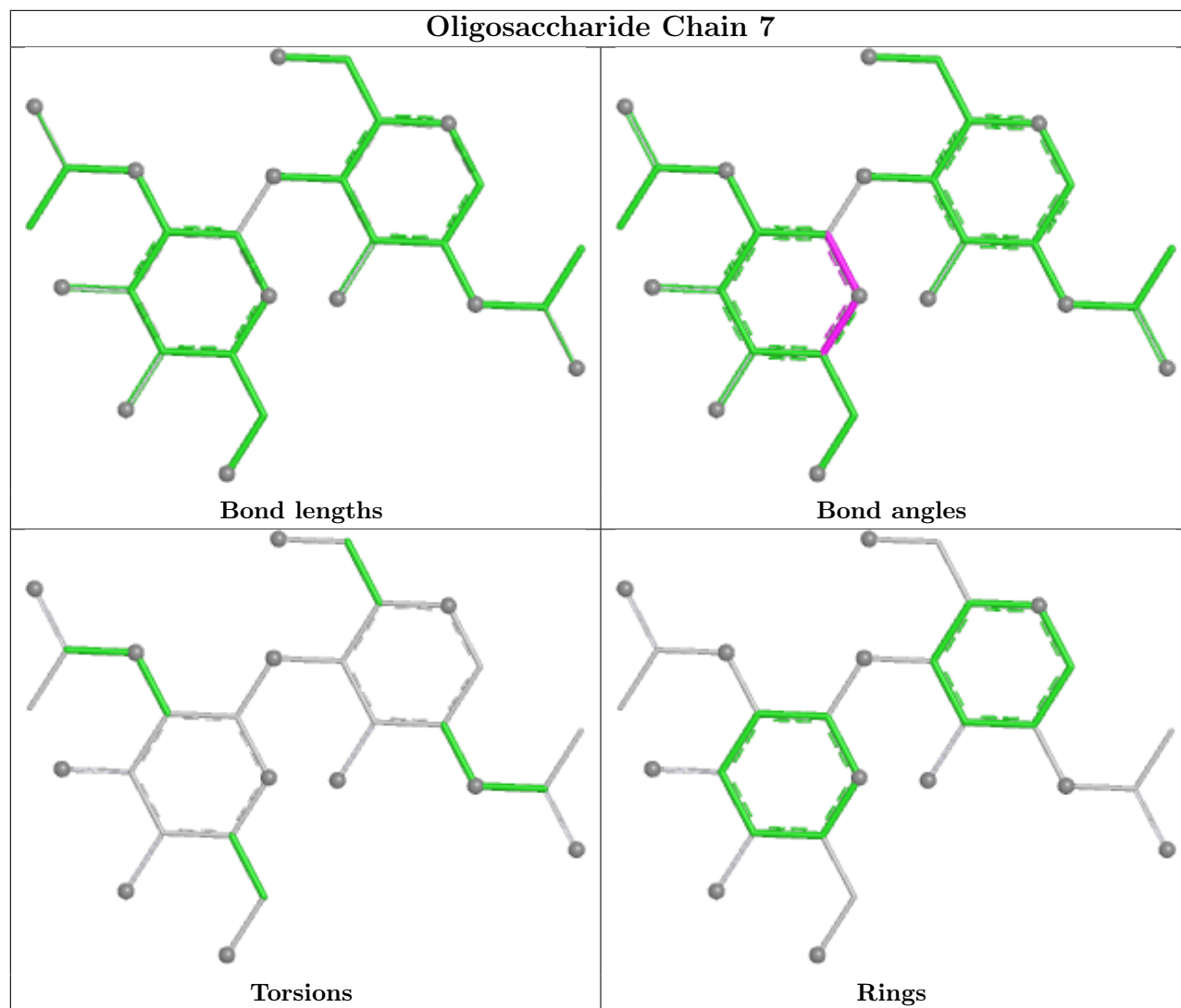


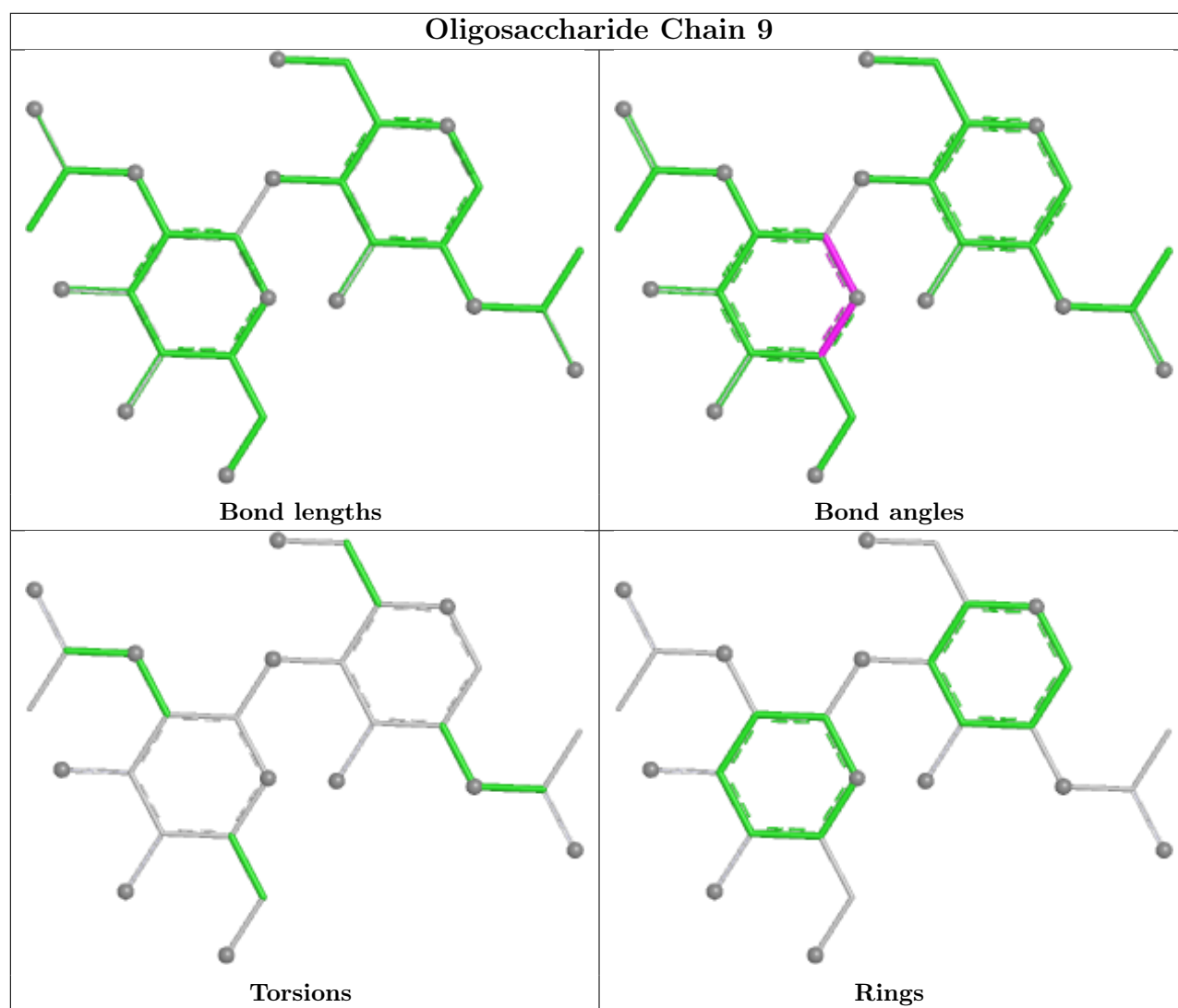


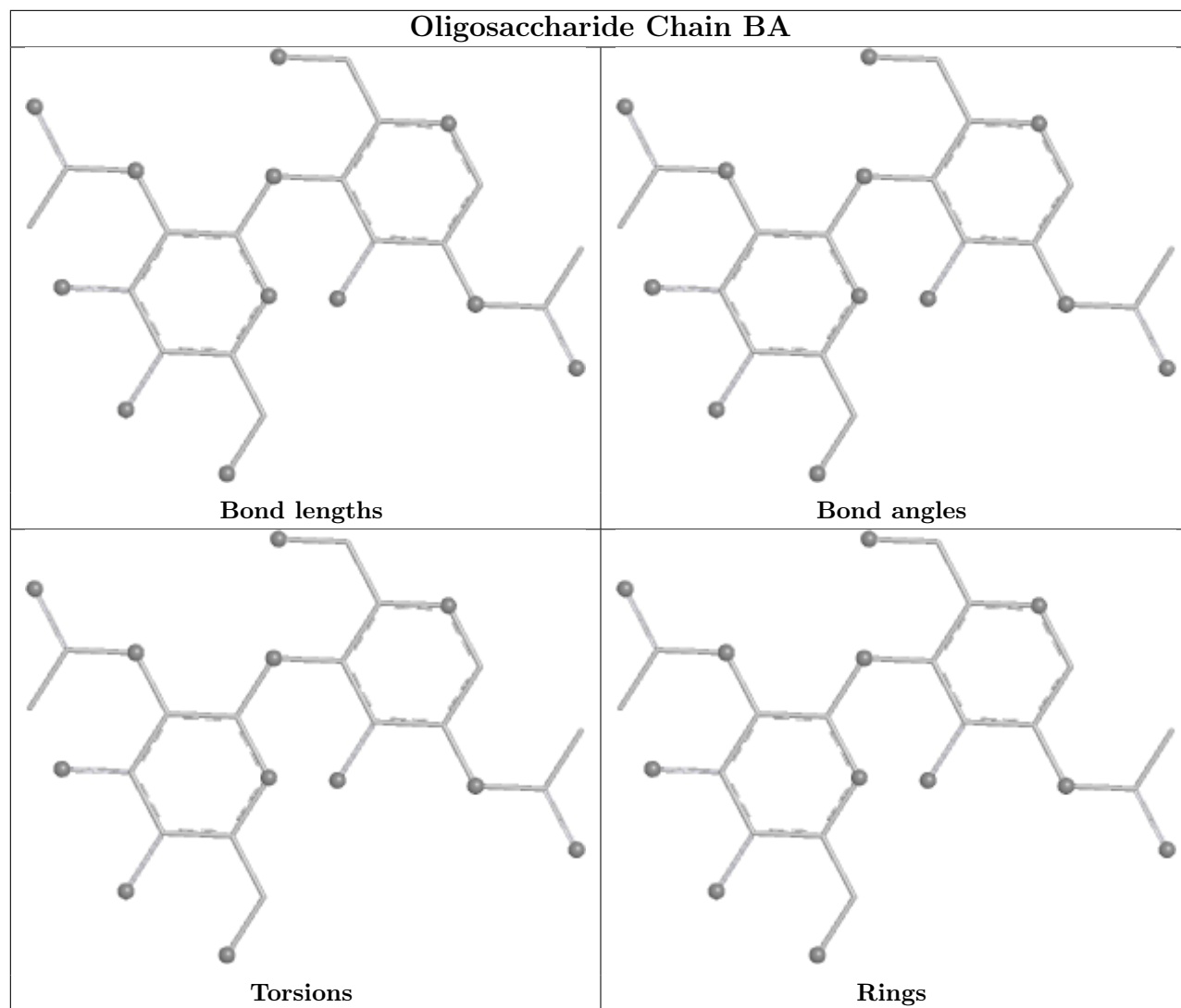


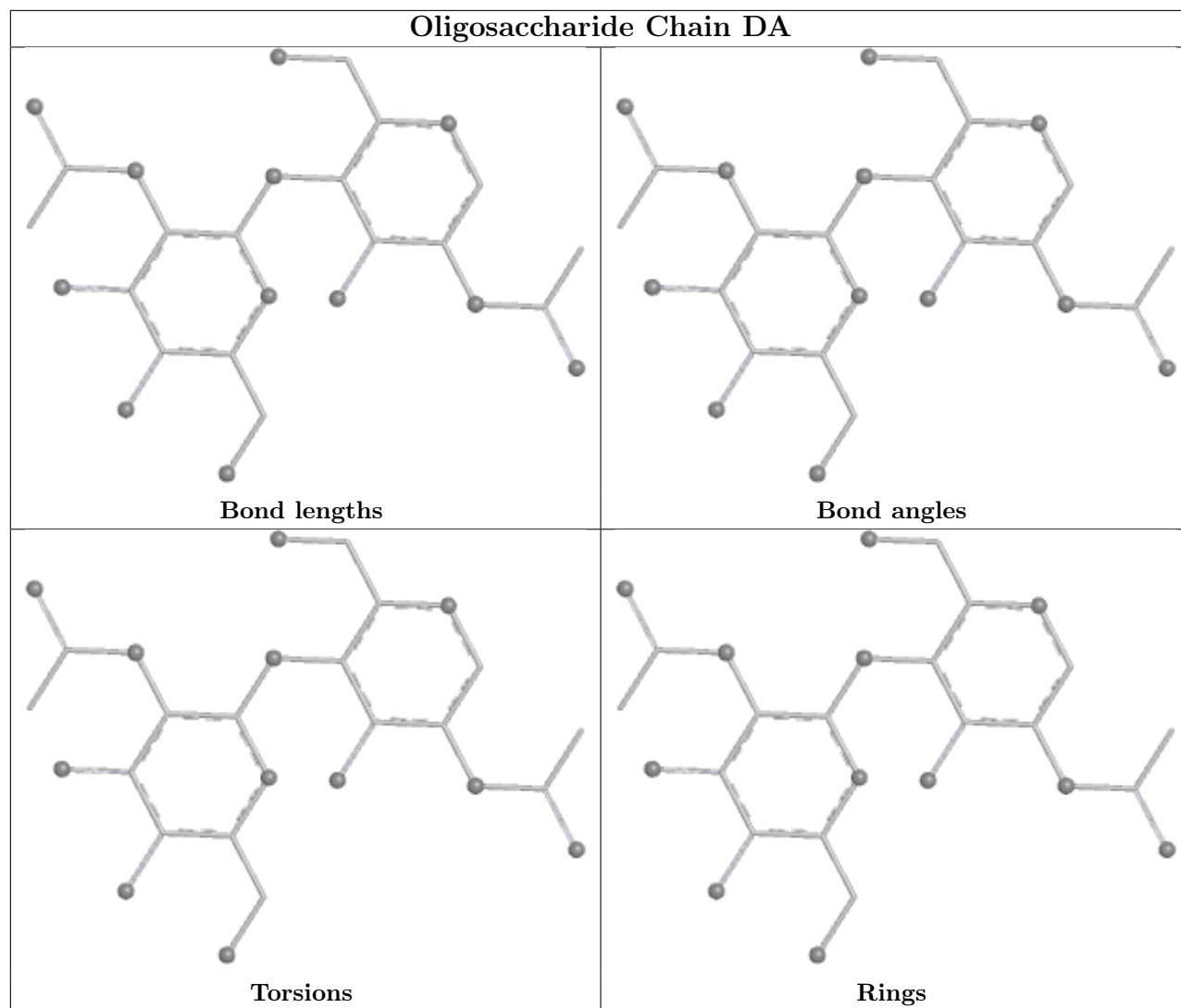


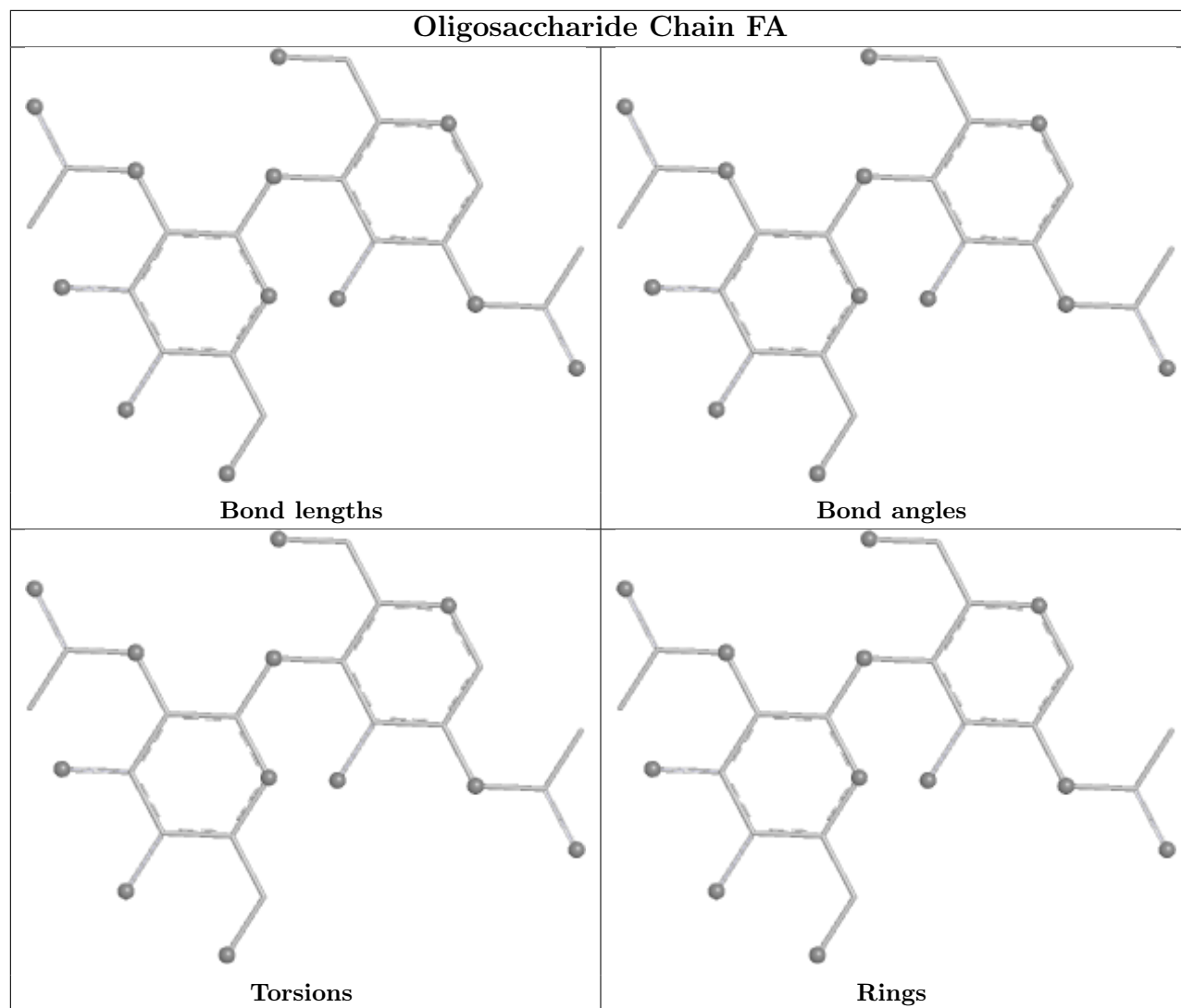


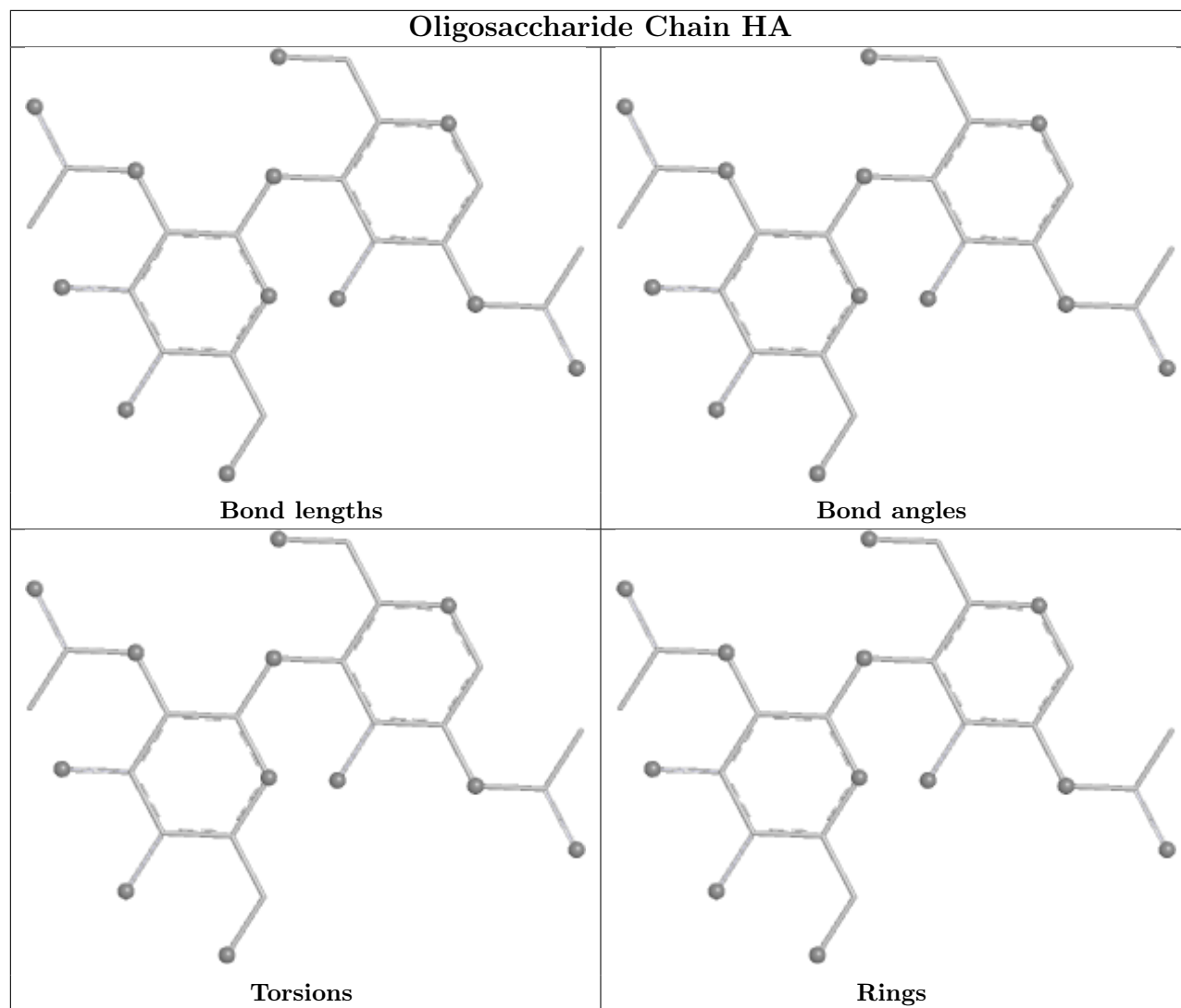


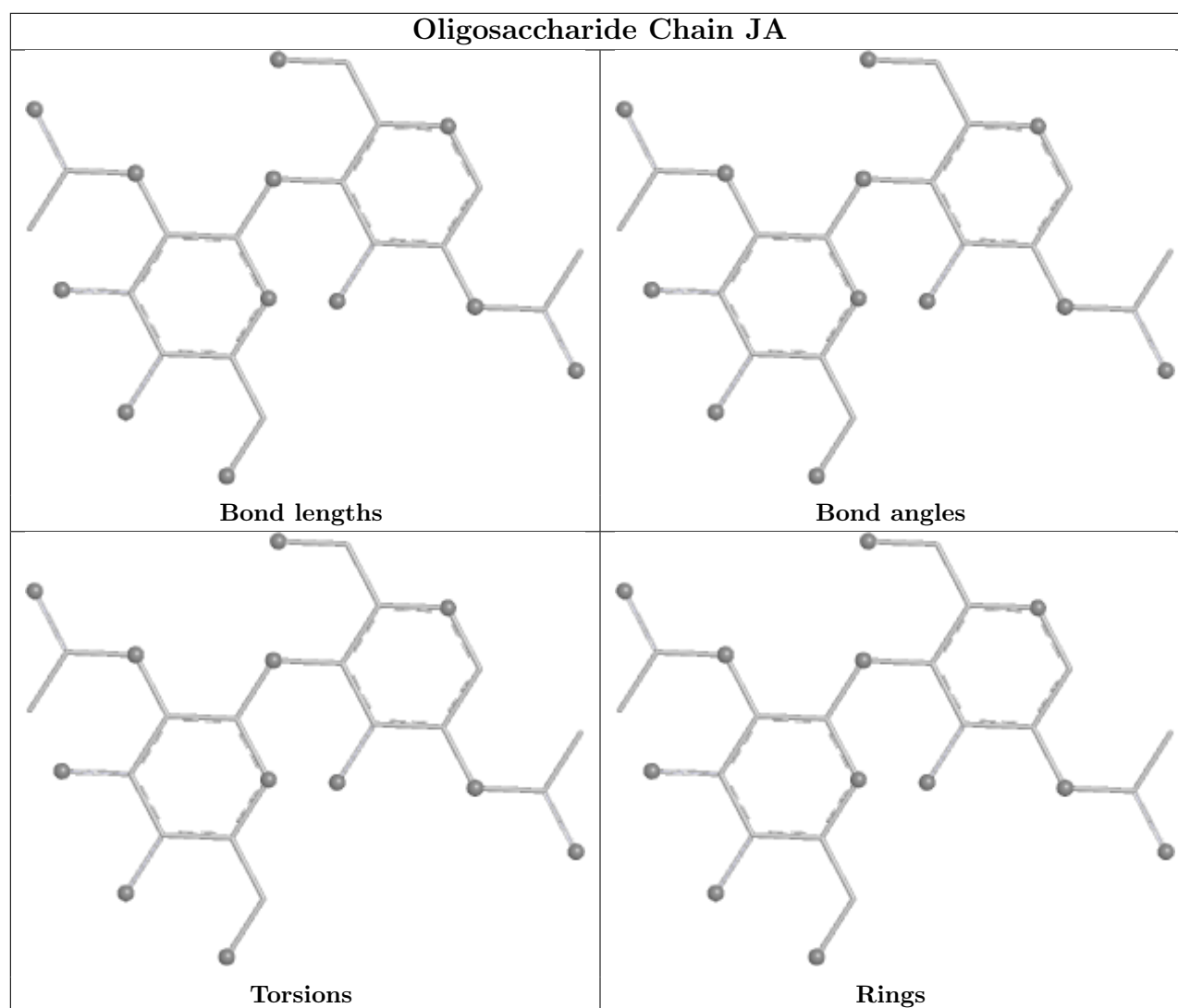












5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	B	201	2	14,14,15	0.62	0	17,19,21	0.87	1 (5%)
7	NAG	N	201	2	14,14,15	0.57	0	17,19,21	1.13	1 (5%)
7	NAG	S	502	1	14,14,15	0.54	0	17,19,21	1.47	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	X	201	2	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
7	NAG	R	201	2	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
7	NAG	L	201	2	14,14,15	0.57	0	17,19,21	0.90	0
7	NAG	V	201	2	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
7	NAG	O	501	1	14,14,15	0.50	0	17,19,21	0.85	0
7	NAG	T	201	2	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
7	NAG	I	501	1	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
7	NAG	Q	501	1	14,14,15	0.43	0	17,19,21	0.99	0
7	NAG	F	201	2	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
7	NAG	J	201	2	14,14,15	0.54	0	17,19,21	1.23	1 (5%)
7	NAG	M	502	1	14,14,15	0.48	0	17,19,21	1.21	2 (11%)
7	NAG	G	502	1	14,14,15	0.50	0	17,19,21	1.15	2 (11%)
7	NAG	M	501	1	14,14,15	0.44	0	17,19,21	1.16	2 (11%)
7	NAG	E	601	1	14,14,15	0.49	0	17,19,21	1.30	2 (11%)
7	NAG	D	201	2	14,14,15	0.54	0	17,19,21	1.18	1 (5%)
7	NAG	C	501	1	14,14,15	0.45	0	17,19,21	1.14	2 (11%)
7	NAG	Q	502	1	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
7	NAG	U	502	1	14,14,15	0.49	0	17,19,21	1.34	2 (11%)
7	NAG	S	501	1	14,14,15	0.46	0	17,19,21	1.19	2 (11%)
7	NAG	G	501	1	14,14,15	0.39	0	17,19,21	1.05	1 (5%)
7	NAG	A	601	1	14,14,15	1.57	2 (14%)	17,19,21	4.36	9 (52%)
7	NAG	W	601	1	14,14,15	0.56	0	17,19,21	1.51	4 (23%)
7	NAG	H	201	2	14,14,15	0.58	0	17,19,21	0.91	1 (5%)
7	NAG	O	502	1	14,14,15	0.52	0	17,19,21	1.30	3 (17%)
7	NAG	P	201	2	14,14,15	0.57	0	17,19,21	0.93	0
7	NAG	U	501	1	14,14,15	0.48	0	17,19,21	0.95	1 (5%)
7	NAG	K	601	1	14,14,15	0.50	0	17,19,21	1.44	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	201	2	-	0/6/23/26	0/1/1/1
7	NAG	N	201	2	-	0/6/23/26	0/1/1/1
7	NAG	S	502	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	X	201	2	-	0/6/23/26	0/1/1/1
7	NAG	R	201	2	-	0/6/23/26	0/1/1/1
7	NAG	L	201	2	-	1/6/23/26	0/1/1/1
7	NAG	V	201	2	-	0/6/23/26	0/1/1/1
7	NAG	O	501	1	-	0/6/23/26	0/1/1/1
7	NAG	T	201	2	-	0/6/23/26	0/1/1/1
7	NAG	I	501	1	-	0/6/23/26	0/1/1/1
7	NAG	Q	501	1	-	0/6/23/26	0/1/1/1
7	NAG	F	201	2	-	0/6/23/26	0/1/1/1
7	NAG	J	201	2	-	0/6/23/26	0/1/1/1
7	NAG	M	502	1	-	0/6/23/26	0/1/1/1
7	NAG	G	502	1	-	0/6/23/26	0/1/1/1
7	NAG	M	501	1	-	0/6/23/26	0/1/1/1
7	NAG	E	601	1	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2	-	0/6/23/26	0/1/1/1
7	NAG	C	501	1	-	2/6/23/26	0/1/1/1
7	NAG	Q	502	1	-	0/6/23/26	0/1/1/1
7	NAG	U	502	1	-	0/6/23/26	0/1/1/1
7	NAG	S	501	1	-	0/6/23/26	0/1/1/1
7	NAG	G	501	1	-	0/6/23/26	0/1/1/1
7	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	NAG	W	601	1	-	0/6/23/26	0/1/1/1
7	NAG	H	201	2	-	0/6/23/26	0/1/1/1
7	NAG	O	502	1	-	0/6/23/26	0/1/1/1
7	NAG	P	201	2	-	0/6/23/26	0/1/1/1
7	NAG	U	501	1	-	0/6/23/26	0/1/1/1
7	NAG	K	601	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	601	NAG	C2-N2	-4.08	1.39	1.46
7	A	601	NAG	C8-C7	-3.50	1.43	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	NAG	O5-C1-C2	-8.89	97.54	111.29
7	A	601	NAG	C2-N2-C7	-8.38	111.67	122.90
7	A	601	NAG	C4-C3-C2	-7.71	99.72	111.02
7	A	601	NAG	C8-C7-N2	-5.99	106.18	116.12
7	A	601	NAG	C3-C4-C5	-4.81	101.51	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	NAG	O3-C3-C2	4.27	118.27	109.40
7	J	201	NAG	C1-O5-C5	4.26	117.90	112.19
7	A	601	NAG	O7-C7-N2	4.14	129.29	121.98
7	D	201	NAG	C1-O5-C5	3.72	117.17	112.19
7	Q	502	NAG	O5-C5-C6	3.35	114.17	107.66
7	K	601	NAG	O5-C5-C6	3.30	114.08	107.66
7	U	502	NAG	O5-C5-C6	3.28	114.04	107.66
7	F	201	NAG	C1-O5-C5	3.03	116.24	112.19
7	W	601	NAG	C1-O5-C5	2.93	116.12	112.19
7	S	502	NAG	O5-C5-C6	2.84	113.19	107.66
7	M	502	NAG	O5-C5-C6	2.81	113.14	107.66
7	R	201	NAG	C1-O5-C5	2.81	115.95	112.19
7	C	501	NAG	C1-O5-C5	2.76	115.88	112.19
7	S	501	NAG	O5-C1-C2	-2.75	107.03	111.29
7	O	502	NAG	O5-C5-C6	2.74	113.00	107.66
7	N	201	NAG	C1-O5-C5	2.73	115.85	112.19
7	S	502	NAG	C4-C3-C2	-2.71	107.05	111.02
7	K	601	NAG	C4-C3-C2	-2.69	107.08	111.02
7	M	501	NAG	C1-O5-C5	2.66	115.75	112.19
7	S	501	NAG	C4-C3-C2	-2.60	107.20	111.02
7	E	601	NAG	O5-C5-C6	2.56	112.65	107.66
7	G	502	NAG	O5-C5-C6	2.54	112.60	107.66
7	W	601	NAG	C4-C3-C2	-2.51	107.34	111.02
7	M	501	NAG	C4-C3-C2	-2.49	107.37	111.02
7	W	601	NAG	O5-C5-C6	2.48	112.48	107.66
7	G	501	NAG	C1-O5-C5	2.46	115.49	112.19
7	C	501	NAG	C4-C3-C2	-2.42	107.47	111.02
7	A	601	NAG	C1-C2-N2	-2.35	106.74	110.43
7	S	502	NAG	O7-C7-C8	-2.34	117.89	122.05
7	U	501	NAG	C4-C3-C2	-2.33	107.60	111.02
7	W	601	NAG	O7-C7-C8	-2.32	117.92	122.05
7	T	201	NAG	C1-O5-C5	2.32	115.29	112.19
7	O	502	NAG	C4-C3-C2	-2.30	107.64	111.02
7	X	201	NAG	C1-O5-C5	2.28	115.24	112.19
7	O	502	NAG	C1-O5-C5	2.25	115.21	112.19
7	G	502	NAG	C4-C3-C2	-2.25	107.72	111.02
7	E	601	NAG	C4-C3-C2	-2.24	107.74	111.02
7	A	601	NAG	C1-O5-C5	-2.22	109.21	112.19
7	Q	502	NAG	O7-C7-C8	-2.17	118.19	122.05
7	V	201	NAG	C1-O5-C5	2.15	115.07	112.19
7	U	502	NAG	C4-C3-C2	-2.14	107.88	111.02
7	M	502	NAG	C4-C3-C2	-2.14	107.88	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	501	NAG	C4-C3-C2	-2.12	107.92	111.02
7	H	201	NAG	C1-O5-C5	2.11	115.02	112.19
7	B	201	NAG	C1-O5-C5	2.05	114.93	112.19
7	K	601	NAG	O7-C7-C8	-2.02	118.45	122.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	NAG	C8-C7-N2-C2
7	A	601	NAG	O7-C7-N2-C2
7	C	501	NAG	C8-C7-N2-C2
7	C	501	NAG	O7-C7-N2-C2
7	L	201	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/323 (98%)	-0.34	0 100 100	17, 39, 68, 127	12 (3%)
1	C	318/323 (98%)	-0.39	0 100 100	15, 42, 70, 106	12 (3%)
1	E	318/323 (98%)	-0.36	1 (0%) 90 79	17, 41, 77, 116	12 (3%)
1	G	318/323 (98%)	-0.42	2 (0%) 85 72	12, 32, 78, 132	12 (3%)
1	I	318/323 (98%)	-0.40	0 100 100	14, 42, 64, 102	12 (3%)
1	K	318/323 (98%)	-0.41	1 (0%) 90 79	16, 42, 61, 112	12 (3%)
1	M	318/323 (98%)	-0.10	2 (0%) 85 72	30, 69, 100, 141	12 (3%)
1	O	318/323 (98%)	-0.22	0 100 100	20, 60, 90, 116	12 (3%)
1	Q	318/323 (98%)	-0.34	0 100 100	21, 48, 72, 115	12 (3%)
1	S	318/323 (98%)	-0.22	2 (0%) 85 72	23, 60, 76, 109	12 (3%)
1	U	318/323 (98%)	-0.39	0 100 100	17, 41, 74, 121	12 (3%)
1	W	318/323 (98%)	-0.32	3 (0%) 81 65	16, 37, 91, 159	12 (3%)
2	B	172/174 (98%)	-0.29	2 (1%) 76 60	18, 60, 97, 111	7 (4%)
2	D	172/174 (98%)	-0.22	0 100 100	22, 58, 81, 85	7 (4%)
2	F	172/174 (98%)	-0.25	1 (0%) 85 72	27, 61, 92, 97	7 (4%)
2	H	172/174 (98%)	-0.22	0 100 100	9, 72, 123, 133	7 (4%)
2	J	172/174 (98%)	-0.21	1 (0%) 85 72	21, 60, 89, 96	7 (4%)
2	L	172/174 (98%)	-0.36	0 100 100	13, 52, 94, 102	7 (4%)
2	N	172/174 (98%)	-0.03	2 (1%) 76 60	21, 85, 125, 133	7 (4%)
2	P	172/174 (98%)	-0.17	1 (0%) 85 72	21, 79, 115, 128	7 (4%)
2	R	172/174 (98%)	-0.32	0 100 100	17, 59, 100, 111	7 (4%)
2	T	172/174 (98%)	-0.17	1 (0%) 85 72	24, 69, 121, 136	7 (4%)
2	V	172/174 (98%)	-0.27	1 (0%) 85 72	19, 55, 102, 115	7 (4%)
2	X	172/174 (98%)	-0.19	1 (0%) 85 72	21, 74, 130, 139	7 (4%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	a	238/241 (98%)	-0.41	0 100 100	13, 37, 62, 74	4 (1%)
3	c	238/241 (98%)	-0.39	0 100 100	15, 36, 54, 59	4 (1%)
3	e	238/241 (98%)	-0.31	1 (0%) 88 76	30, 66, 75, 83	4 (1%)
3	g	238/241 (98%)	-0.30	0 100 100	12, 39, 95, 107	4 (1%)
3	i	238/241 (98%)	-0.46	0 100 100	12, 30, 59, 70	4 (1%)
3	k	238/241 (98%)	-0.20	4 (1%) 69 52	31, 65, 91, 107	4 (1%)
3	m	238/241 (98%)	-0.27	1 (0%) 88 76	22, 47, 73, 86	4 (1%)
3	o	238/241 (98%)	-0.13	2 (0%) 82 66	40, 85, 107, 124	4 (1%)
3	q	238/241 (98%)	-0.29	0 100 100	22, 54, 81, 91	4 (1%)
3	s	238/241 (98%)	-0.18	3 (1%) 75 58	37, 81, 100, 126	4 (1%)
3	u	238/241 (98%)	-0.41	1 (0%) 88 76	29, 56, 74, 86	4 (1%)
3	w	238/241 (98%)	-0.38	1 (0%) 88 76	18, 46, 83, 97	4 (1%)
4	b	213/214 (99%)	-0.42	0 100 100	13, 28, 62, 66	1 (0%)
4	d	213/214 (99%)	-0.46	0 100 100	19, 39, 67, 73	1 (0%)
4	f	213/214 (99%)	-0.46	0 100 100	27, 54, 86, 97	1 (0%)
4	h	213/214 (99%)	-0.43	1 (0%) 87 74	17, 33, 85, 91	1 (0%)
4	j	213/214 (99%)	-0.48	0 100 100	16, 31, 66, 80	1 (0%)
4	l	213/214 (99%)	-0.34	0 100 100	32, 79, 103, 107	1 (0%)
4	n	213/214 (99%)	-0.46	1 (0%) 87 74	31, 44, 54, 60	1 (0%)
4	p	213/214 (99%)	-0.14	4 (1%) 66 50	39, 79, 105, 111	1 (0%)
4	r	213/214 (99%)	-0.35	0 100 100	24, 53, 68, 73	1 (0%)
4	t	213/214 (99%)	-0.38	0 100 100	32, 68, 105, 115	1 (0%)
4	v	213/214 (99%)	-0.45	0 100 100	21, 48, 84, 93	1 (0%)
4	x	213/214 (99%)	-0.50	0 100 100	25, 41, 54, 59	1 (0%)
All	All	11292/11424 (98%)	-0.32	40 (0%) 88 76	9, 51, 98, 159	288 (2%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	o	133	GLY	4.9
3	s	133	GLY	4.2
1	S	319	GLY	3.8
2	P	16	GLY	3.7
1	M	13	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	181	GLY	3.2
2	J	97	GLU	3.2
4	h	110	VAL	3.0
2	B	33	GLY	3.0
1	G	24[A]	THR	2.8
3	k	188	SER	2.8
3	w	144	ASP	2.6
1	M	12	THR	2.5
1	W	9	PRO	2.5
3	o	190	GLY	2.4
2	X	44	ALA	2.4
4	n	164	THR	2.4
2	N	29	SER	2.4
1	S	82	GLU	2.3
2	F	57	GLU	2.3
2	T	168	ASN	2.3
1	W	37	THR	2.3
2	V	122	THR	2.3
3	s	53	GLY	2.3
3	k	137	ALA	2.3
1	K	231	SER	2.3
4	p	63	SER	2.3
2	B	1	GLY	2.2
3	k	53	GLY	2.2
4	p	187	GLU	2.2
3	k	138	LEU	2.1
1	E	124	GLY	2.1
3	s	7	SER	2.1
3	e	8	GLY	2.1
4	p	157	GLY	2.1
4	p	60	SER	2.1
3	u	144	ASP	2.0
2	N	63	PHE	2.0
1	W	225	GLY	2.0
3	m	100(D)	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PCA	o	1	8/9	0.92	0.07	77,78,79,79	0
3	PCA	k	1	8/9	0.93	0.09	50,52,54,57	0
3	PCA	i	1	8/9	0.94	0.11	32,32,33,33	0
3	PCA	u	1	8/9	0.94	0.11	54,55,56,56	0
3	PCA	a	1	8/9	0.95	0.08	36,36,37,38	0
3	PCA	e	1	8/9	0.96	0.11	54,56,59,62	0
3	PCA	g	1	8/9	0.97	0.09	35,36,38,38	0
3	PCA	q	1	8/9	0.97	0.09	57,57,58,58	0
3	PCA	s	1	8/9	0.97	0.07	63,64,64,64	0
3	PCA	m	1	8/9	0.97	0.07	40,41,41,41	0
3	PCA	c	1	8/9	0.98	0.06	36,37,38,39	0
3	PCA	w	1	8/9	0.98	0.07	27,27,27,29	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	Y	1	14/15	-	-	45,48,60,61	0
5	NAG	Y	2	14/15	-	-	45,54,65,65	0
5	BMA	Y	3	11/12	-	-	70,74,78,78	0
5	MAN	Y	4	11/12	-	-	78,80,84,84	0
5	NAG	y	1	14/15	-	-	30,32,34,34	0
5	NAG	y	2	14/15	-	-	32,34,37,40	0
5	BMA	y	3	11/12	-	-	44,48,51,53	0
5	MAN	y	4	11/12	-	-	56,59,60,61	0
5	NAG	0	1	14/15	-	-	40,46,56,56	0
5	NAG	0	2	14/15	-	-	46,50,58,60	0
5	BMA	0	3	11/12	-	-	64,68,72,73	0
5	MAN	0	4	11/12	-	-	76,78,80,81	0
5	NAG	2	1	14/15	-	-	26,32,41,42	0
5	NAG	2	2	14/15	-	-	30,37,45,47	0
5	BMA	2	3	11/12	-	-	51,55,58,60	0
5	MAN	2	4	11/12	-	-	62,65,66,67	0
5	NAG	4	1	14/15	-	-	40,47,57,58	0
5	NAG	4	2	14/15	-	-	42,50,60,62	0
5	BMA	4	3	11/12	-	-	65,69,73,73	0
5	MAN	4	4	11/12	-	-	75,78,80,80	0
5	NAG	6	1	14/15	-	-	49,56,67,67	0
5	NAG	6	2	14/15	-	-	51,60,69,71	0

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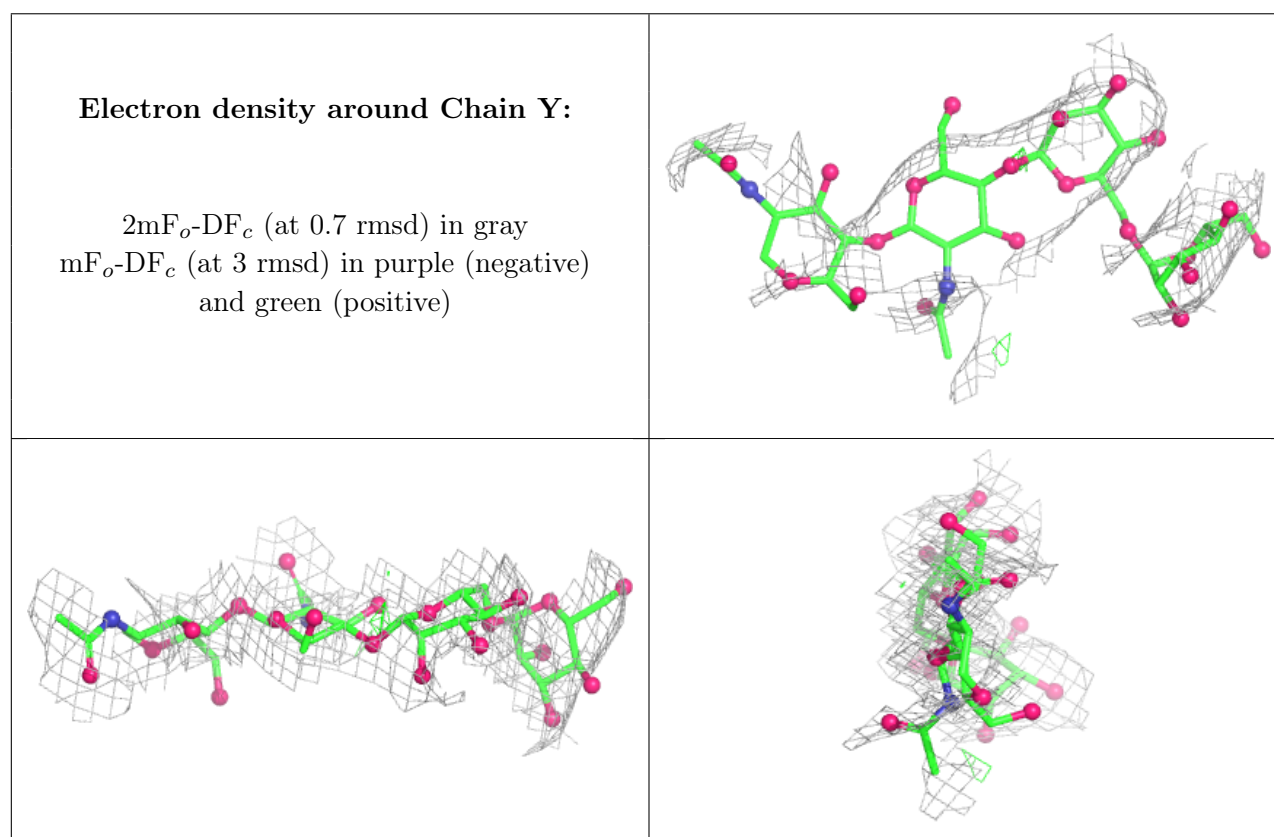
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	6	3	11/12	-	-	75,79,82,83	0
5	MAN	6	4	11/12	-	-	84,87,89,90	0
5	NAG	8	1	14/15	-	-	66,67,68,68	0
5	NAG	8	2	14/15	-	-	66,69,71,74	0
5	BMA	8	3	11/12	-	-	78,82,85,86	0
5	MAN	8	4	11/12	-	-	88,92,93,93	0
5	NAG	AA	1	14/15	-	-	43,49,57,58	0
5	NAG	AA	2	14/15	-	-	47,52,59,62	0
5	BMA	AA	3	11/12	-	-	66,70,72,75	0
5	MAN	AA	4	11/12	-	-	78,81,81,82	0
5	NAG	CA	1	14/15	-	-	54,60,70,71	0
5	NAG	CA	2	14/15	-	-	57,66,77,78	0
5	BMA	CA	3	11/12	-	-	82,87,91,92	0
5	MAN	CA	4	11/12	-	-	92,96,98,98	0
5	NAG	EA	1	14/15	-	-	53,58,69,69	0
5	NAG	EA	2	14/15	-	-	52,58,68,69	0
5	BMA	EA	3	11/12	-	-	72,75,77,79	0
5	MAN	EA	4	11/12	-	-	81,83,84,84	0
5	NAG	GA	1	14/15	-	-	41,43,48,48	0
5	NAG	GA	2	14/15	-	-	44,46,55,58	0
5	BMA	GA	3	11/12	-	-	62,67,72,72	0
5	MAN	GA	4	11/12	-	-	74,78,81,82	0
5	NAG	IA	1	14/15	-	-	39,46,56,57	0
5	NAG	IA	2	14/15	-	-	43,52,61,63	0
5	BMA	IA	3	11/12	-	-	68,73,76,76	0
5	MAN	IA	4	11/12	-	-	78,81,84,84	0
6	NAG	Z	1	14/15	-	-	37,40,44,49	0
6	NAG	Z	2	14/15	-	-	51,59,65,65	0
6	NAG	z	1	14/15	-	-	43,45,49,50	0
6	NAG	z	2	14/15	-	-	45,52,59,60	0
6	NAG	1	1	14/15	-	-	60,66,70,74	0
6	NAG	1	2	14/15	-	-	75,83,89,90	0
6	NAG	3	1	14/15	-	-	37,42,47,49	0
6	NAG	3	2	14/15	-	-	49,58,66,66	0
6	NAG	5	1	14/15	-	-	50,57,61,63	0
6	NAG	5	2	14/15	-	-	62,74,81,82	0
6	NAG	7	1	14/15	-	-	40,47,50,53	0
6	NAG	7	2	14/15	-	-	54,62,69,69	0
6	NAG	9	1	14/15	-	-	70,73,76,76	0
6	NAG	9	2	14/15	-	-	70,79,89,89	0
6	NAG	BA	1	14/15	-	-	71,77,82,84	0
6	NAG	BA	2	14/15	-	-	82,93,102,102	0

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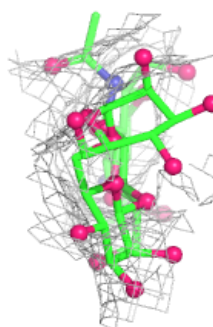
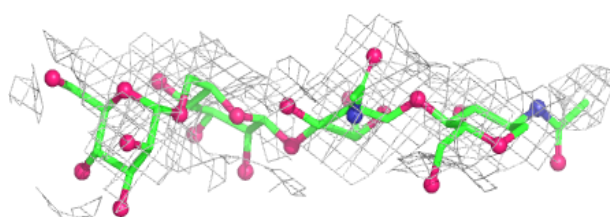
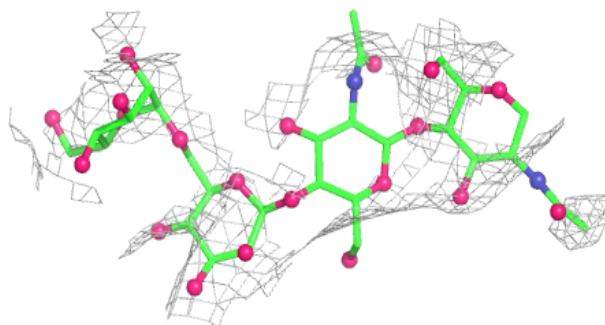
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	DA	1	14/15	-	-	46,50,54,57	0
6	NAG	DA	2	14/15	-	-	59,67,73,73	0
6	NAG	FA	1	14/15	-	-	59,63,67,70	0
6	NAG	FA	2	14/15	-	-	70,80,86,87	0
6	NAG	HA	1	14/15	-	-	42,44,47,47	0
6	NAG	HA	2	14/15	-	-	48,56,62,63	0
6	NAG	JA	1	14/15	-	-	53,60,66,68	0
6	NAG	JA	2	14/15	-	-	67,78,86,87	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

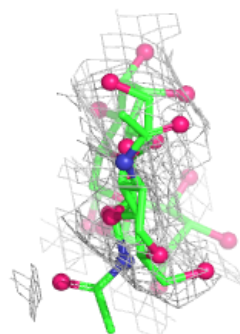
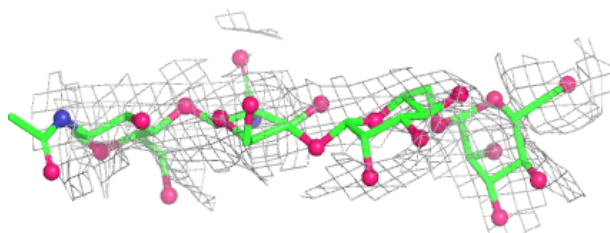
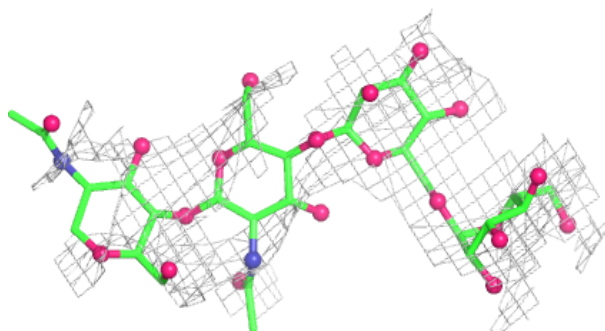


Electron density around Chain y:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

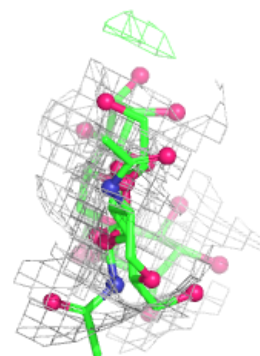
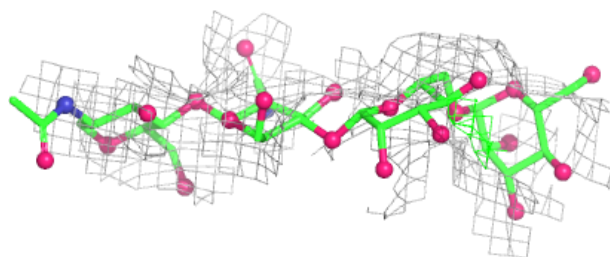
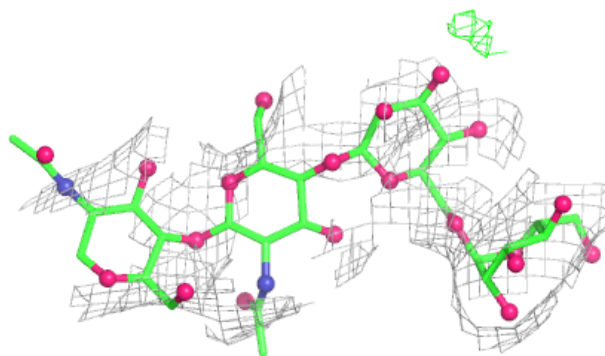
**Electron density around Chain 0:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

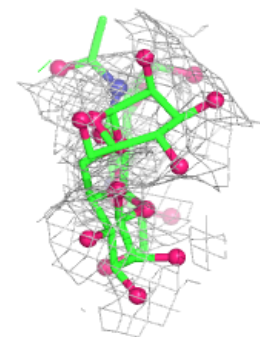
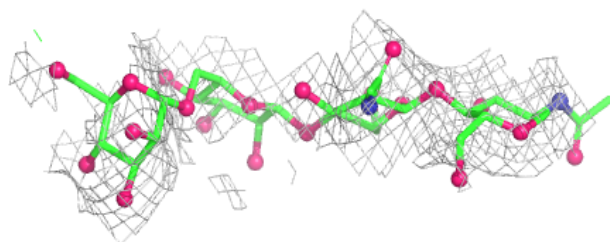
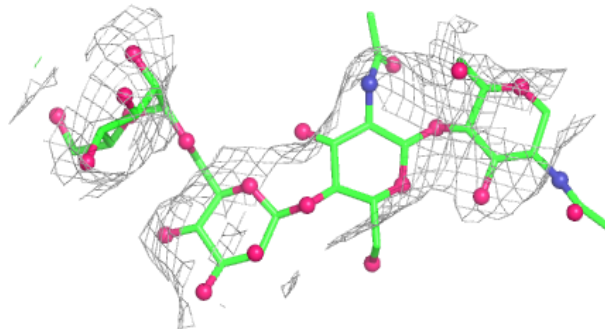


Electron density around Chain 2:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

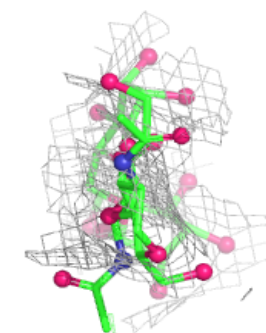
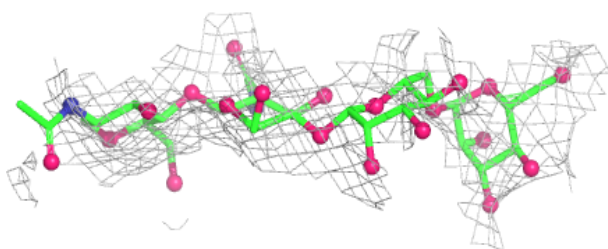
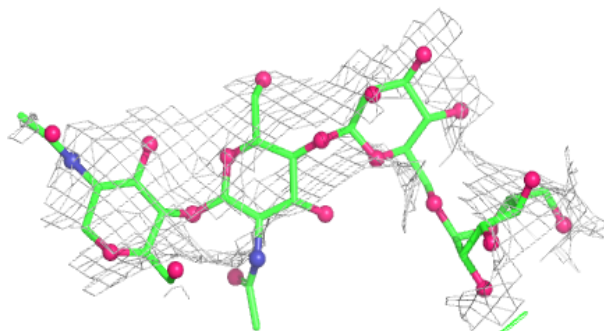
**Electron density around Chain 4:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

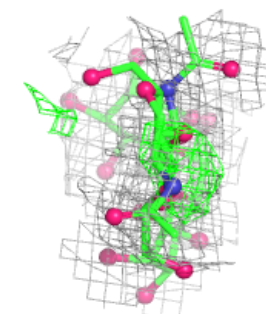
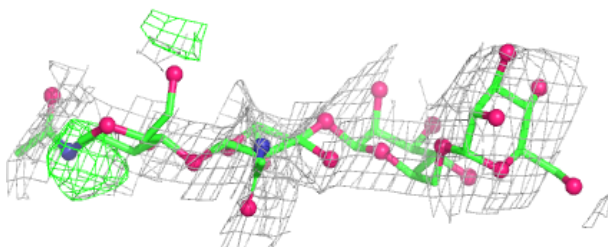
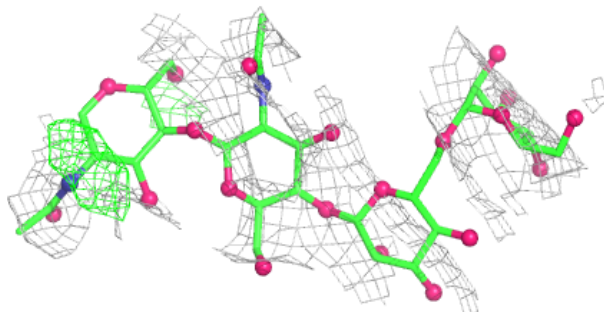


Electron density around Chain 6:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

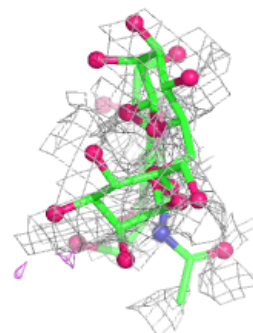
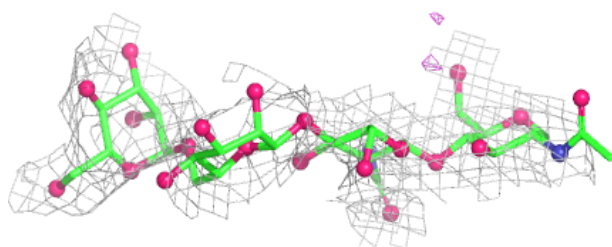
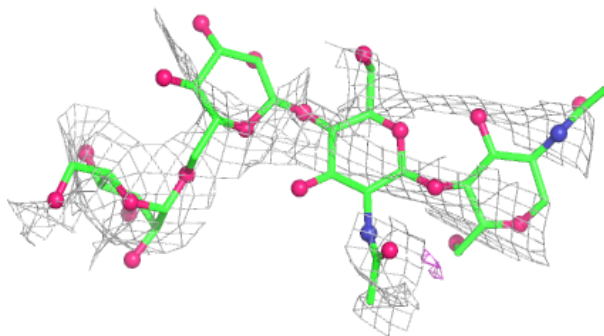
**Electron density around Chain 8:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

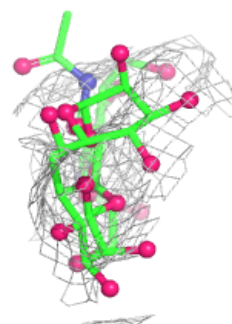
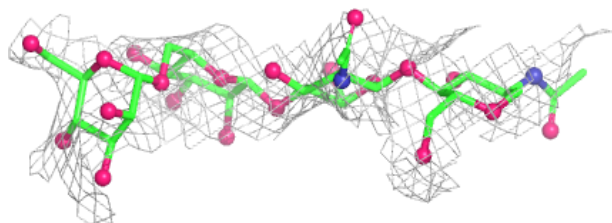
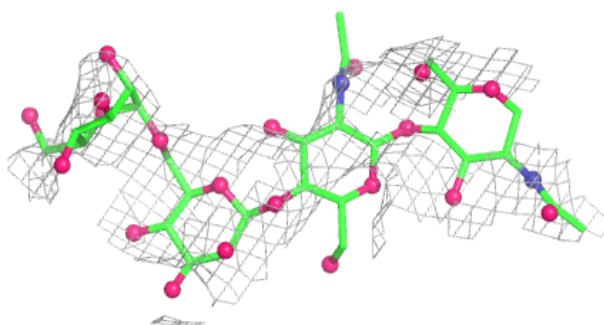


Electron density around Chain AA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

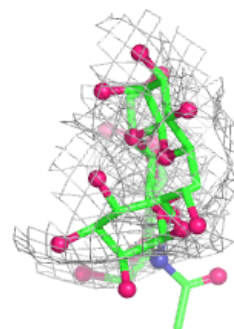
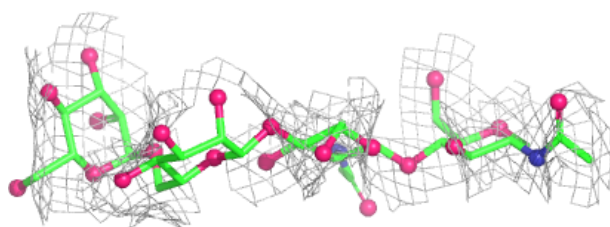
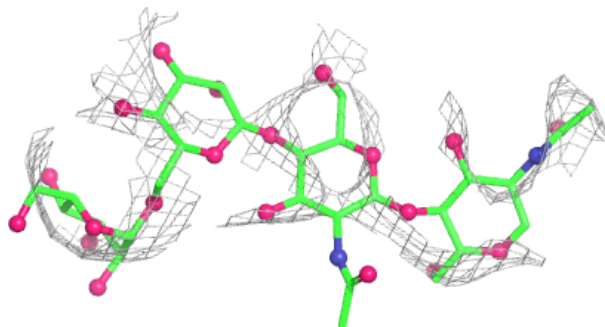
**Electron density around Chain CA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

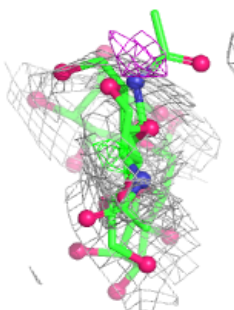
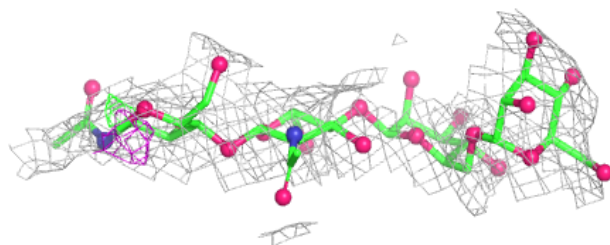
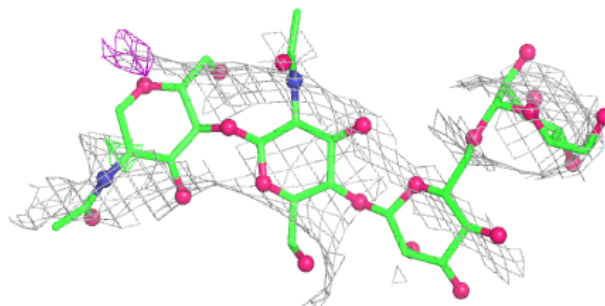


Electron density around Chain EA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

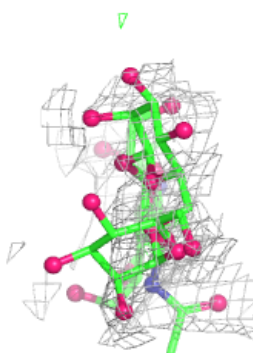
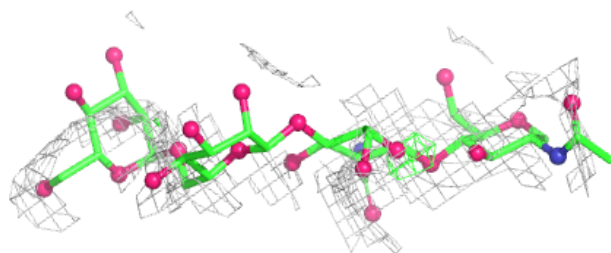
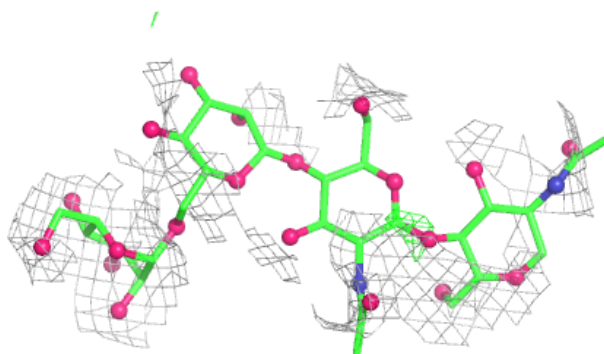
**Electron density around Chain GA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

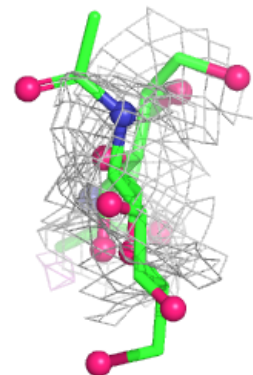
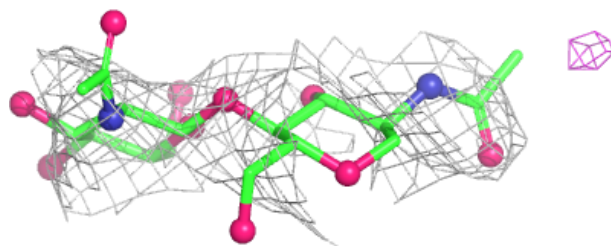
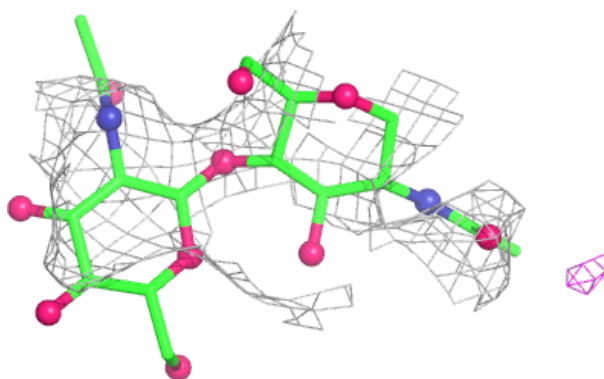


Electron density around Chain IA:

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and green (positive)

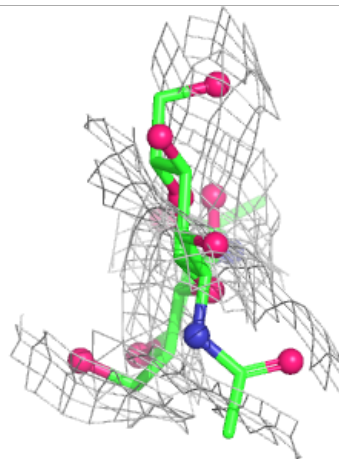
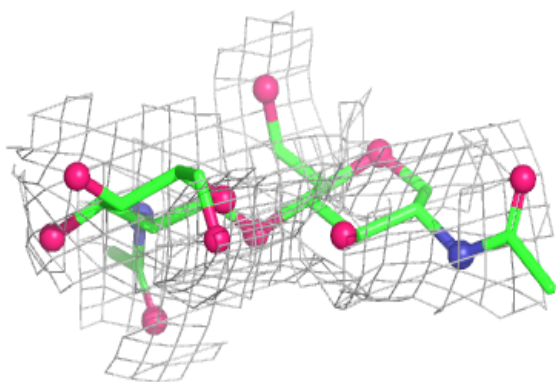
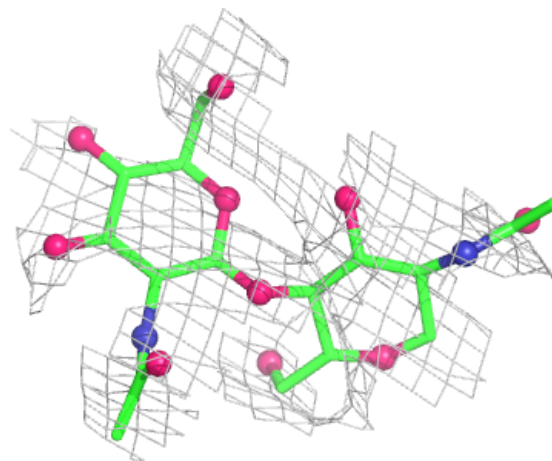
**Electron density around Chain Z:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



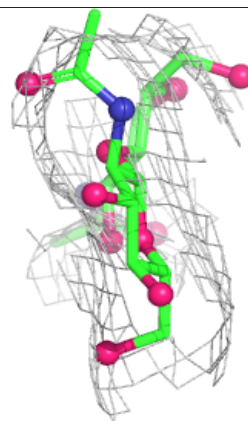
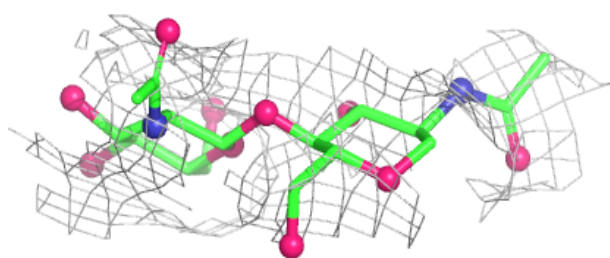
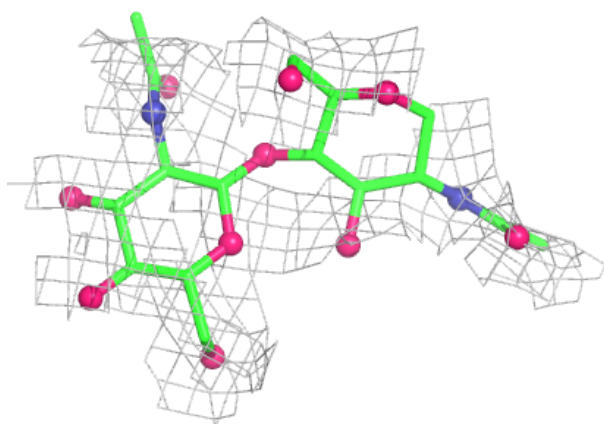
Electron density around Chain z:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

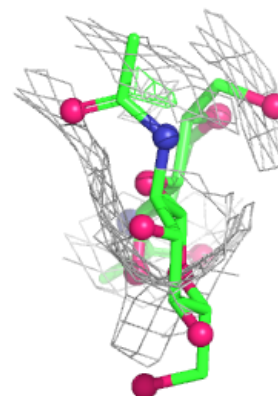
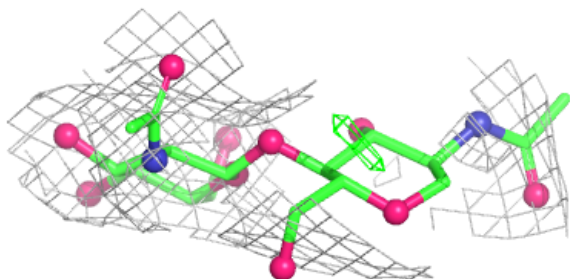
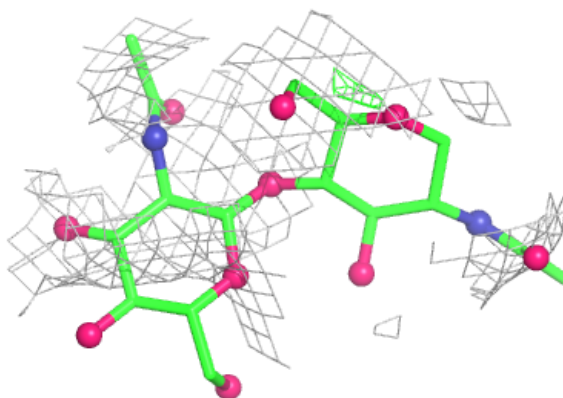


Electron density around Chain 1:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

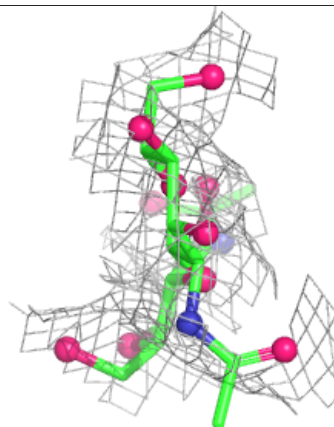
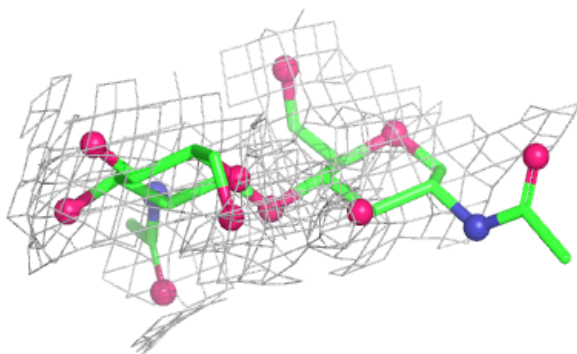
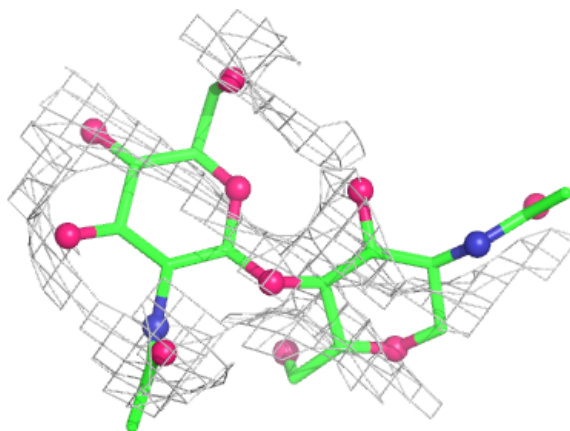
**Electron density around Chain 3:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



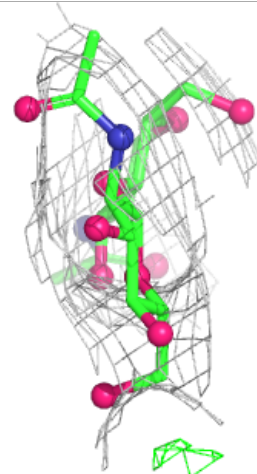
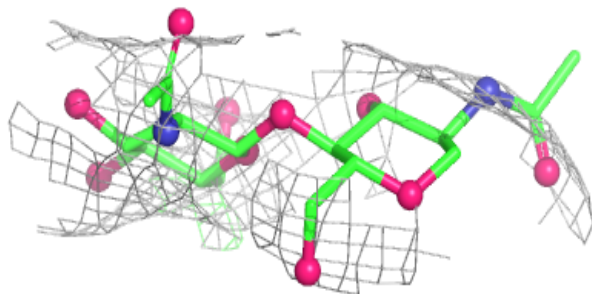
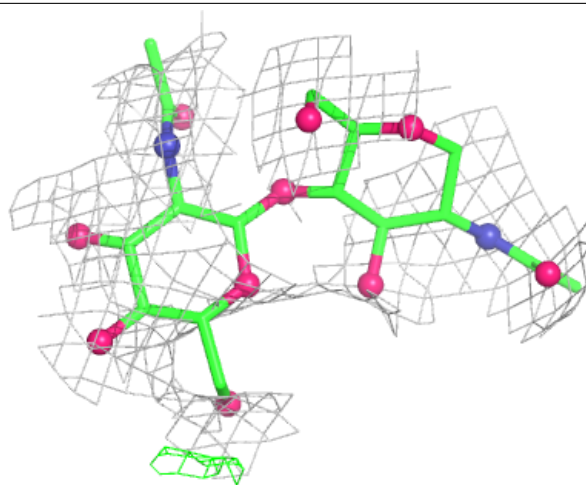
Electron density around Chain 5:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



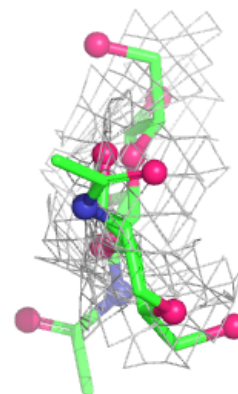
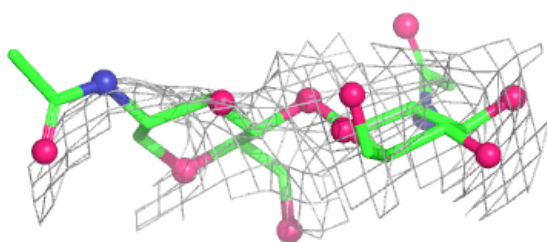
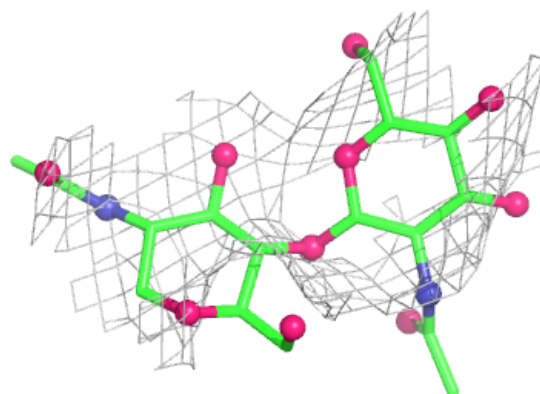
Electron density around Chain 7:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

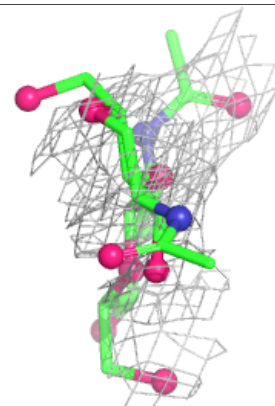
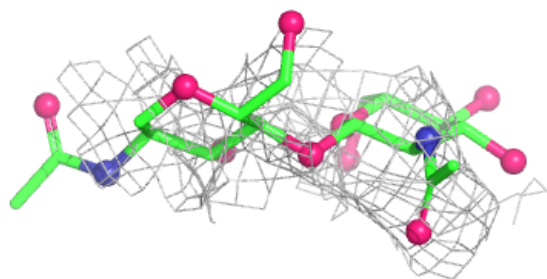
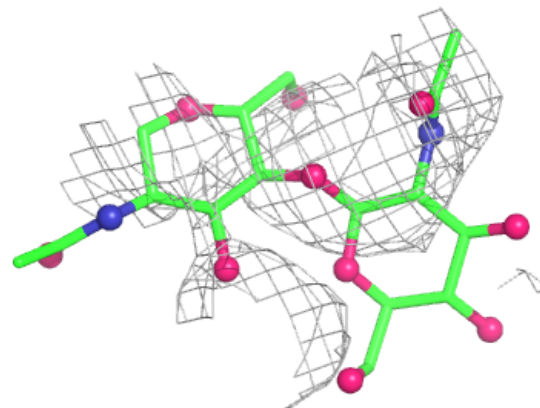


Electron density around Chain 9:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
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and green (positive)

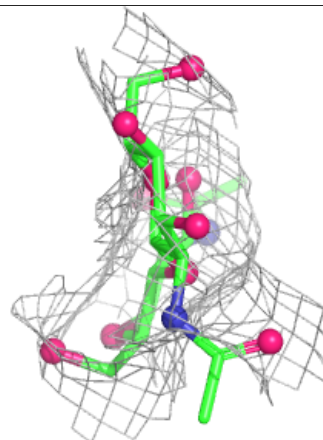
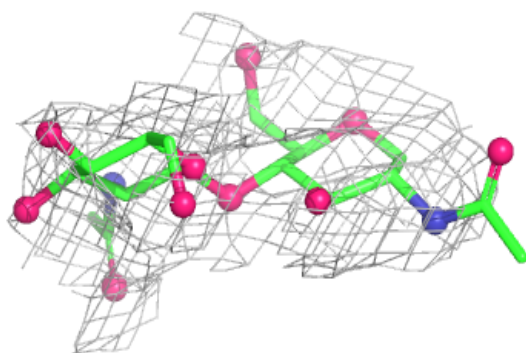
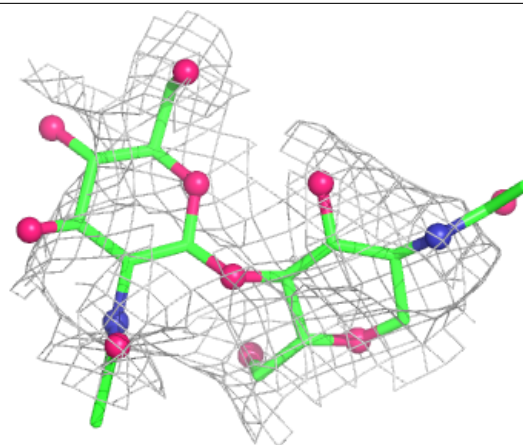
**Electron density around Chain BA:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



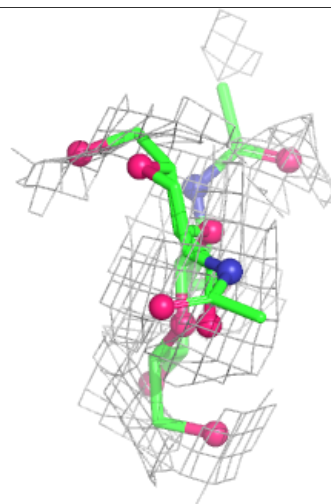
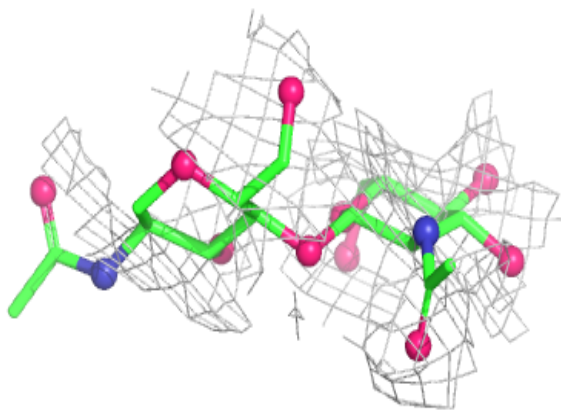
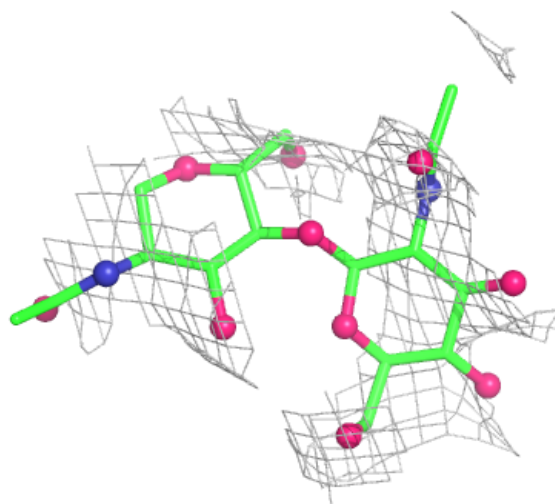
Electron density around Chain DA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



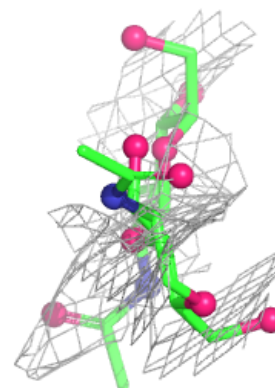
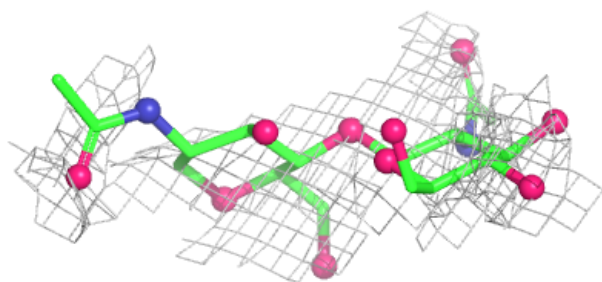
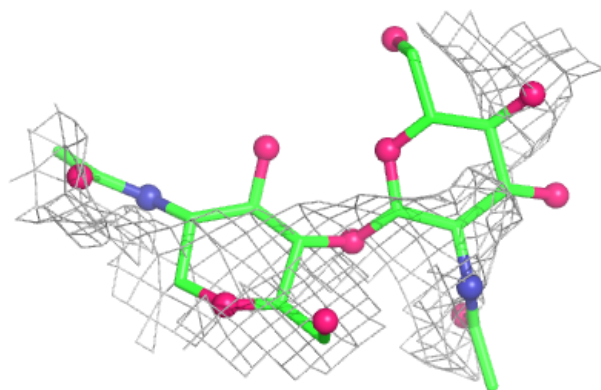
Electron density around Chain FA:

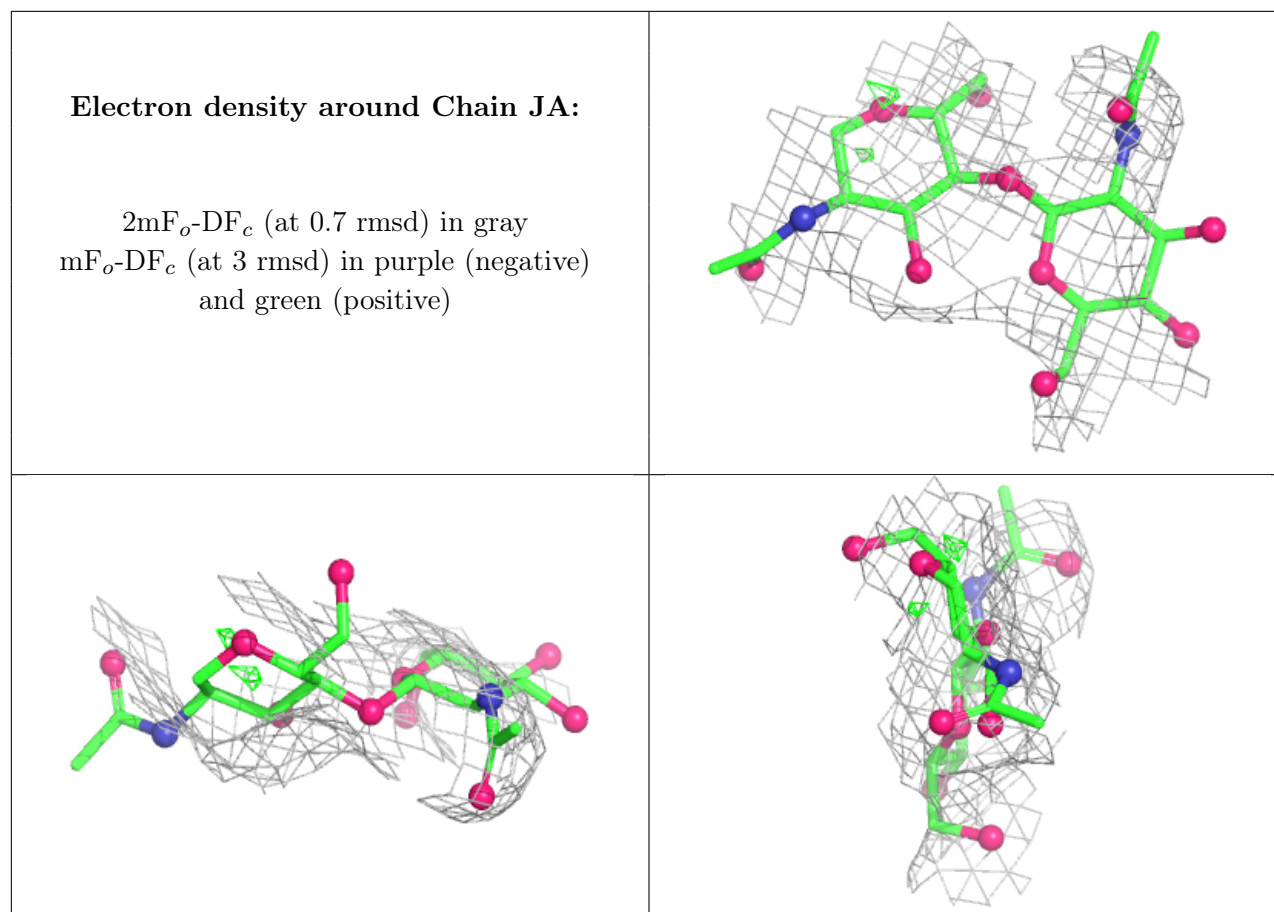
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain HA:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	N	201	14/15	0.92	0.11	109,114,121,122	0
7	NAG	M	501	14/15	0.93	0.12	89,92,96,98	0
7	NAG	E	601	14/15	0.94	0.11	59,64,66,67	0
7	NAG	F	201	14/15	0.94	0.12	88,93,99,100	0
7	NAG	J	201	14/15	0.94	0.13	73,75,79,80	0
7	NAG	A	601	14/15	0.94	0.13	38,44,45,46	0
7	NAG	C	501	14/15	0.94	0.11	66,69,74,76	0
7	NAG	Q	501	14/15	0.94	0.09	66,74,80,83	0
7	NAG	R	201	14/15	0.94	0.09	100,111,117,117	0
7	NAG	T	201	14/15	0.94	0.14	93,100,105,107	0
7	NAG	U	501	14/15	0.94	0.10	66,70,75,78	0
7	NAG	K	601	14/15	0.95	0.10	58,64,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	S	501	14/15	0.95	0.10	71,78,84,87	0
7	NAG	D	201	14/15	0.95	0.11	73,75,77,78	0
7	NAG	Q	502	14/15	0.95	0.09	61,67,70,71	0
7	NAG	U	502	14/15	0.95	0.11	46,48,50,51	0
7	NAG	L	201	14/15	0.96	0.10	81,89,95,96	0
7	NAG	O	501	14/15	0.96	0.11	90,98,105,108	0
7	NAG	S	502	14/15	0.96	0.10	65,69,74,75	0
7	NAG	P	201	14/15	0.96	0.08	96,101,106,107	0
7	NAG	G	502	14/15	0.96	0.12	42,47,49,51	0
7	NAG	M	502	14/15	0.96	0.11	75,76,77,78	0
7	NAG	V	201	14/15	0.96	0.09	83,85,91,93	0
7	NAG	G	501	14/15	0.97	0.08	68,75,84,87	0
7	NAG	O	502	14/15	0.97	0.08	74,78,81,83	0
7	NAG	H	201	14/15	0.97	0.08	115,125,133,134	0
7	NAG	W	601	14/15	0.97	0.09	45,51,52,54	0
7	NAG	X	201	14/15	0.97	0.10	119,129,138,140	0
7	NAG	B	201	14/15	0.99	0.06	80,89,94,96	0
7	NAG	I	501	14/15	0.99	0.08	66,74,81,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.